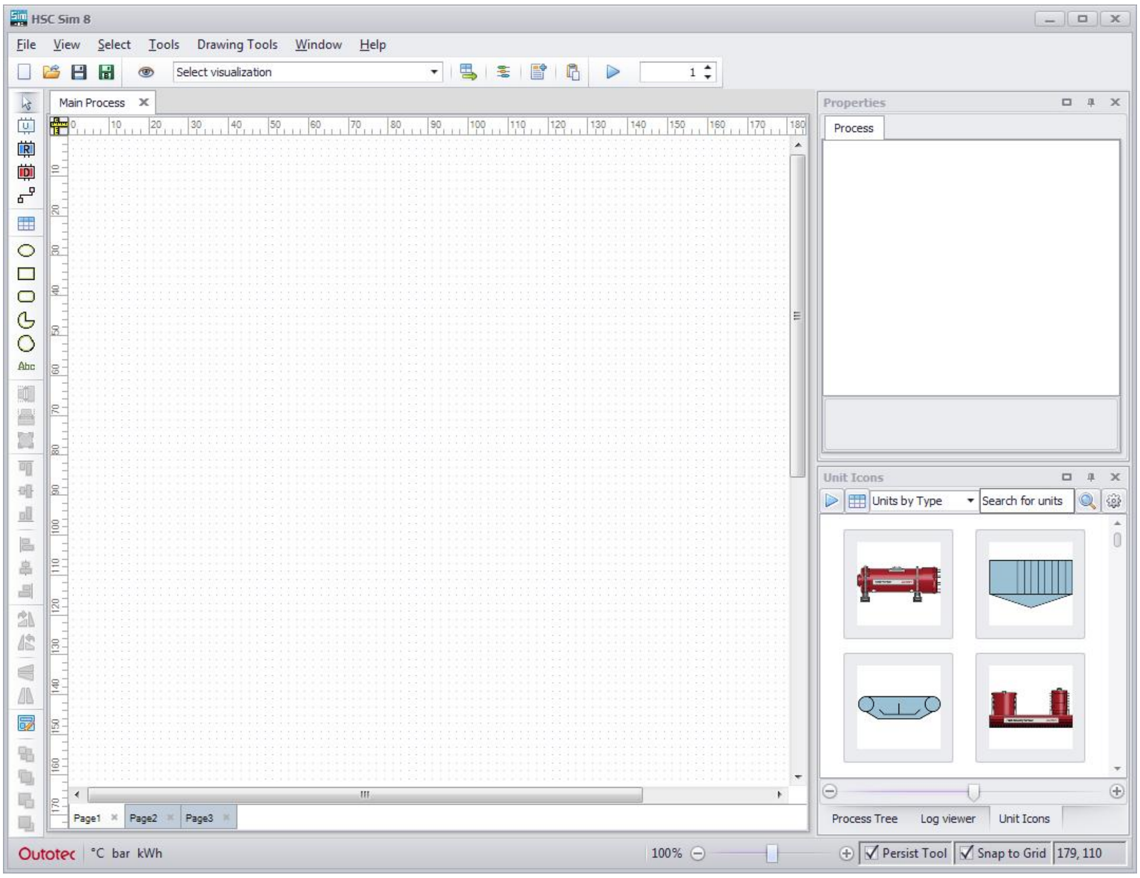
Research Center, Pori / Petri Kobylin, Lauri Mäenpää, Matti Hietala, Jussi-Pekka Kentala

40. Sim Module - Common Tools



40.1. Drawing flowsheets and adding tables to flowsheets

This chapter explains how to draw and add tables to a flowsheet. In addition to the instructions chapter, the user should also read unit-specific Chapters 41-47 of this manual before running the simulations (41- 42 Distribution Units, 43-44 Reactions Units, 45-46 Minerals Processing Units and 47 Converter Units, which are needed if different units are combined in the flowsheet).

The most important icons for drawing are:

Fig. 1. Icons for drawing Units and Streams, where the first icon is Select, U = Generic Units, R = Reactions Units, D = Distributions Units, and the last icon is Streams.

40.1.1. Drawing units

Select the unit by left-clicking the unit icon. The cursor shows the user which icon is active. Move the cursor to somewhere on the flowsheet and draw a unit by a) holding down the left mouse button b) moving the mouse to increase the size of the unit c) releasing the button to stop drawing, see **Fig. 2**. The user can change the size of the units later.

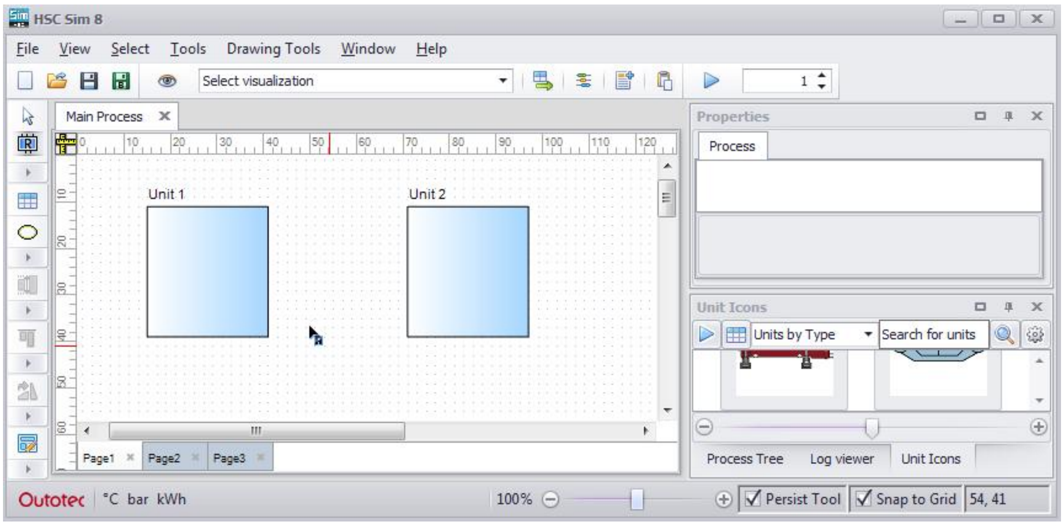


Fig. 2. Drawing two Reactions (Hydro) units. The Reactions unit is the active icon in this figure, see the mouse cursor.

40.1.2. Drawing streams

Select the stream icon with the mouse (left button). Move the cursor to somewhere on the flowsheet and click the mouse (left button) to start the stream. The user can add a corner to the stream with another click and double-click (left button) to end the drawing of the stream, see **Fig. 3**.

<u>Editing Streams</u>

How to a) make a corner on the stream b) change the angle of the stream and c) remove the corners of the stream d) change the input and output units of the stream e) check the connection of the streams.

a) Choose the Select icon and by holding down the **shift** + **left mouse button,** the user can make corners on the streams by moving the mouse.

b) Choose the Select icon and click the stream to see the nodes (blue squares). Hold down the mouse button on a node and move the mouse to change the angle of the stream.

c) Choose the Select icon, select the stream, then select one stream node (blue square), move one node on top of another node to remove a stream corner.

d) Choose the Select icon and move the beginning or end of the stream to a new unit or out of the unit. HSC8 Sim will suggest a new connection to the stream that the user can accept (OK) or Cancel.

e) When the flowsheet is ready, check that the streams are connected to the correct units. The user can check connections visually, see **Fig. 4**. A white circle or arrow means that the stream source or destination is unknown (a gray arrow means it is known). Blue stream means input, black stream is between two units and red stream means output. It is also possible to click the **Tools** menu to show the **process tree**. The most time-consuming task is selecting streams one by one and looking at the **properties** (process sheet) to see the source and destination of the stream.

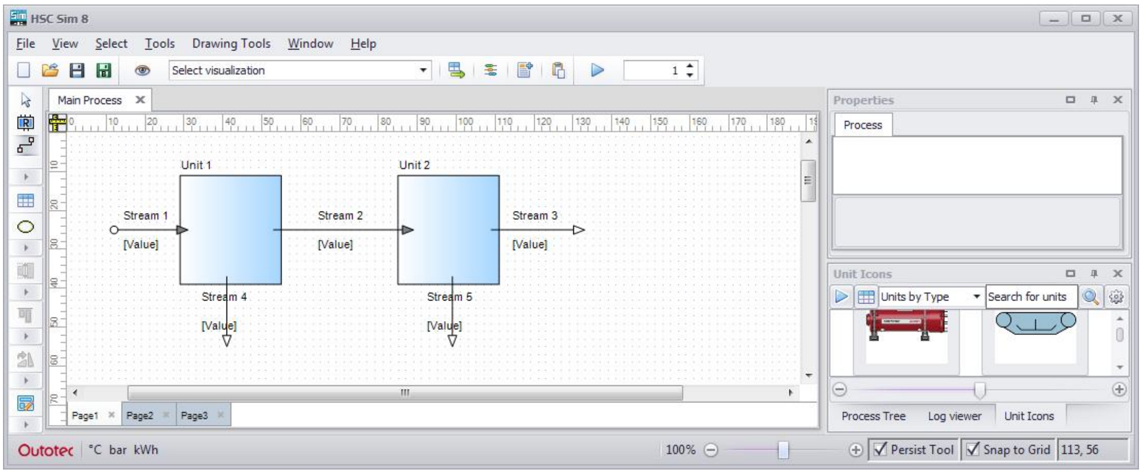


Fig. 3. Drawing streams.

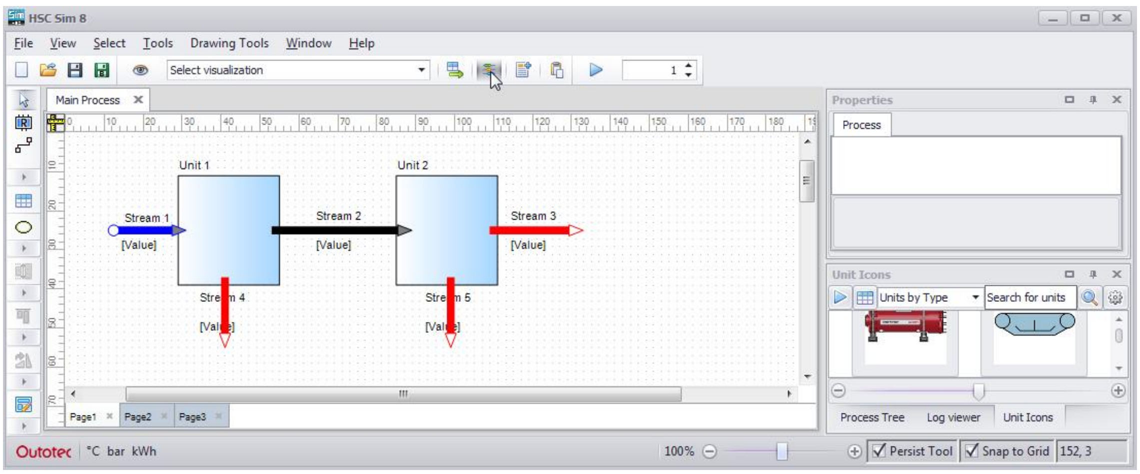


Fig. 4. Visualizing stream connections.

40.1.3. Renaming units and streams

Choose the Select icon and rename units and streams by double-clicking the name or click the name label and edit properties (process sheet) - NameID cell, see **Fig. 5**.

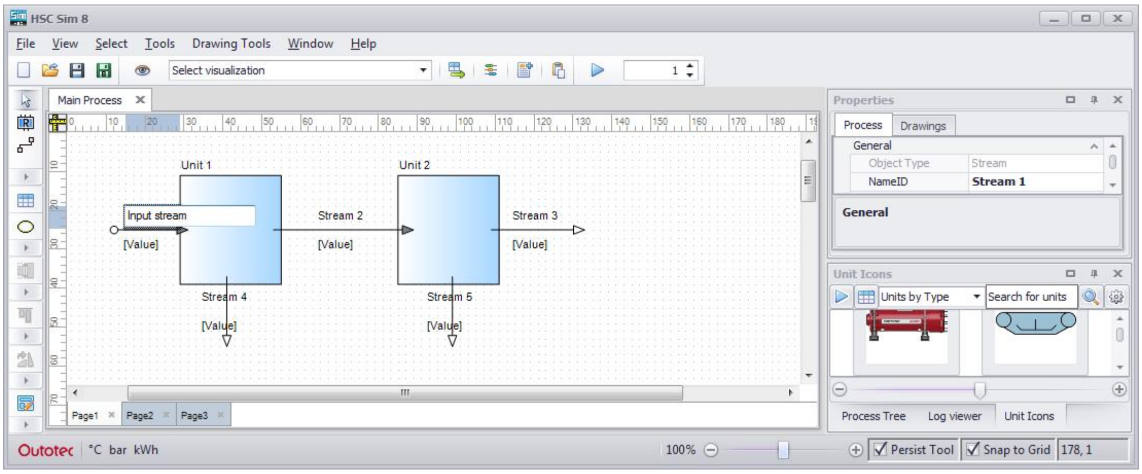


Fig. 5. Renaming units and streams.

40.1.4. Inserting tables and stream tables (typically done after simulations)

The user can add **tables** to visualize important parameters of the results. Choose the Table icon and draw the table in the same way as you draw the units. The user can open table editor by double-clicking the table, where the user can add more rows and columns. It is important to uncheck **Size lock** when adjusting the table size. It is typical to use this table to show a summary of the results. The user can insert header labels and add any process values as cell references in this table (copy cell reference from the unit sheets and paste cell reference in the table), see **Fig. 6** and **Fig. 7**.

The user can also insert **stream tables** by clicking the Stream Table Editor icon, which will open the editor where the user can add variables (by double-clicking). A visible variable list can be sorted by dragging the variables up and down in the list, see **Fig. 8**. The user can check which stream tables can be visible or invisible in the editor or does that later from **View Menu**...stream tables...show/hide all.

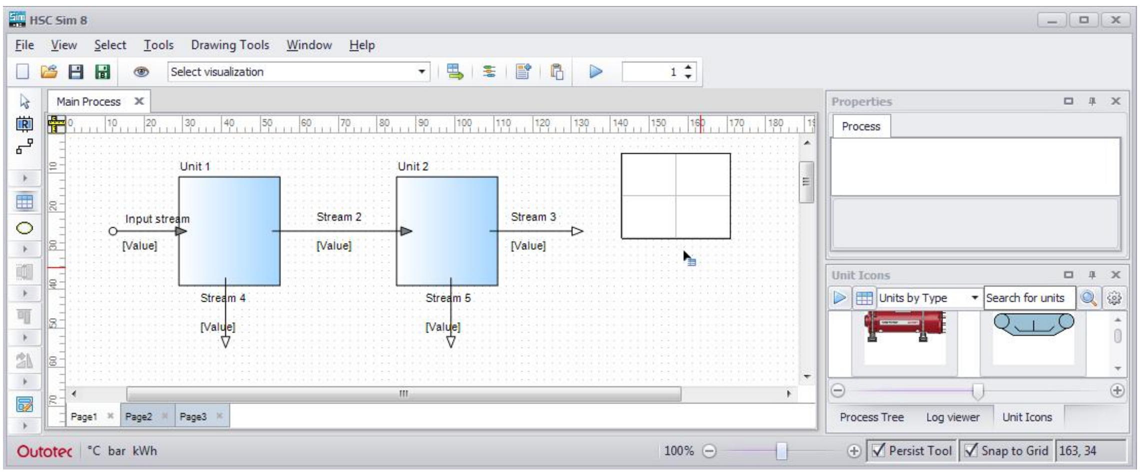


Fig. 6. Table added to the flowsheet.

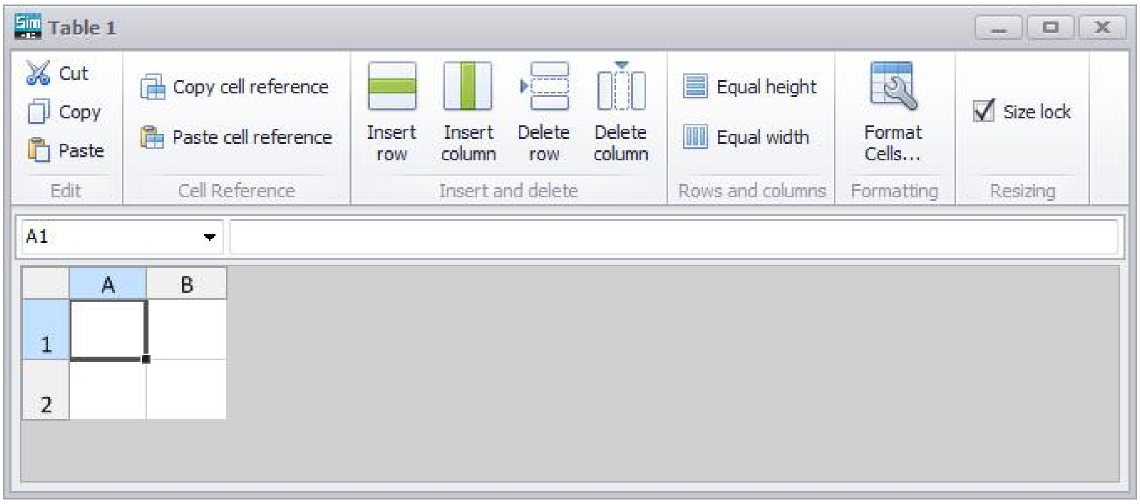


Fig. 7. Table editor, remember to uncheck **Size lock** when inserting rows and columns.

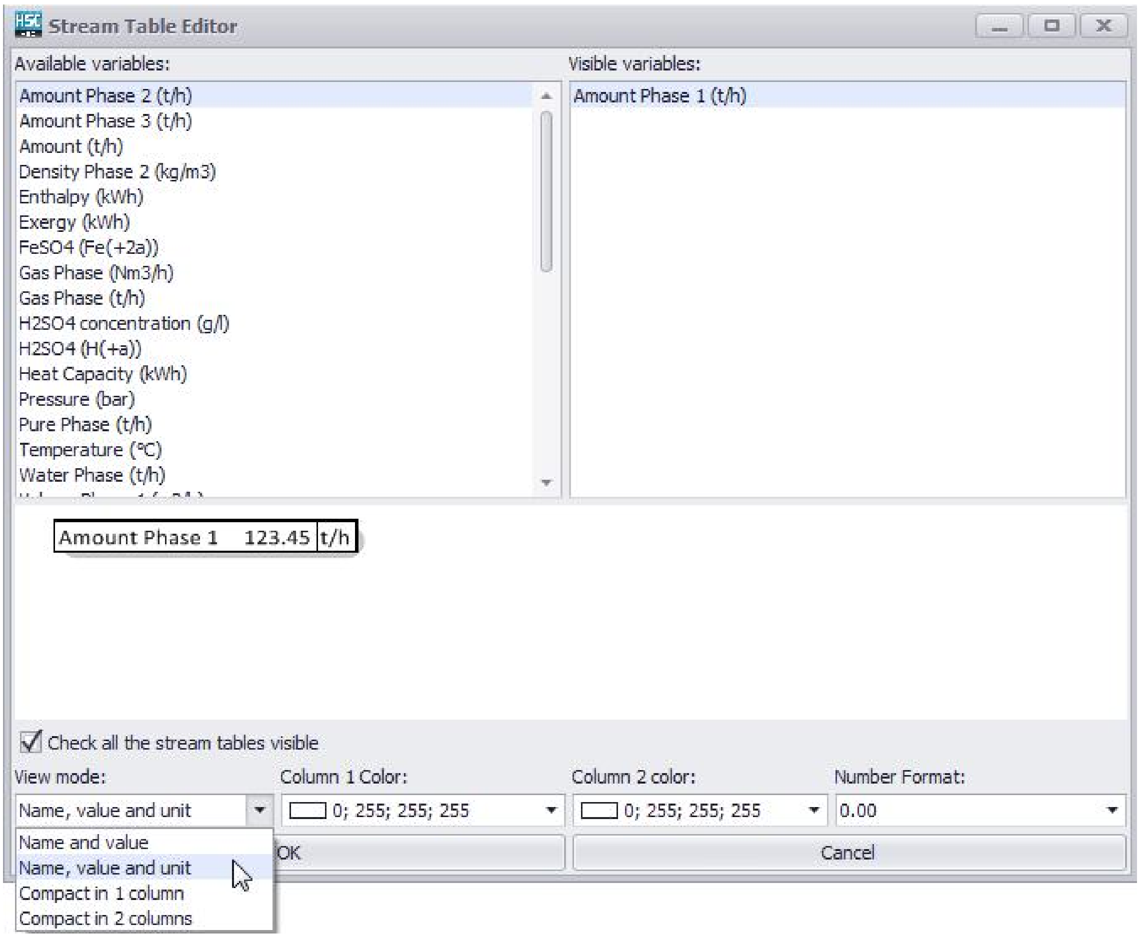


Fig. 8. Stream tables editor for adding stream tables to the flowsheet. Add and remove variables by double-clicking.

40.1.5. Editing a flowsheet

Sometimes the user wants to edit a flowsheet later and add new units. Adding a new unit (Unit 3) in the middle of a stream (Stream 1) connected to two units (Unit 1 and Unit 2) is explained here. First, draw a new unit (Unit 3) and connect Stream 1 from Unit 1 to Unit 3. Then add a new stream (Stream 2), which starts from Unit 3 and ends at Unit 2, see **Fig. 9** - **Fig. 11**. Information in Unit 1 and Unit 2 is automatically updated so the user only needs to make changes in Unit 3 and Stream 3 to run the simulation.

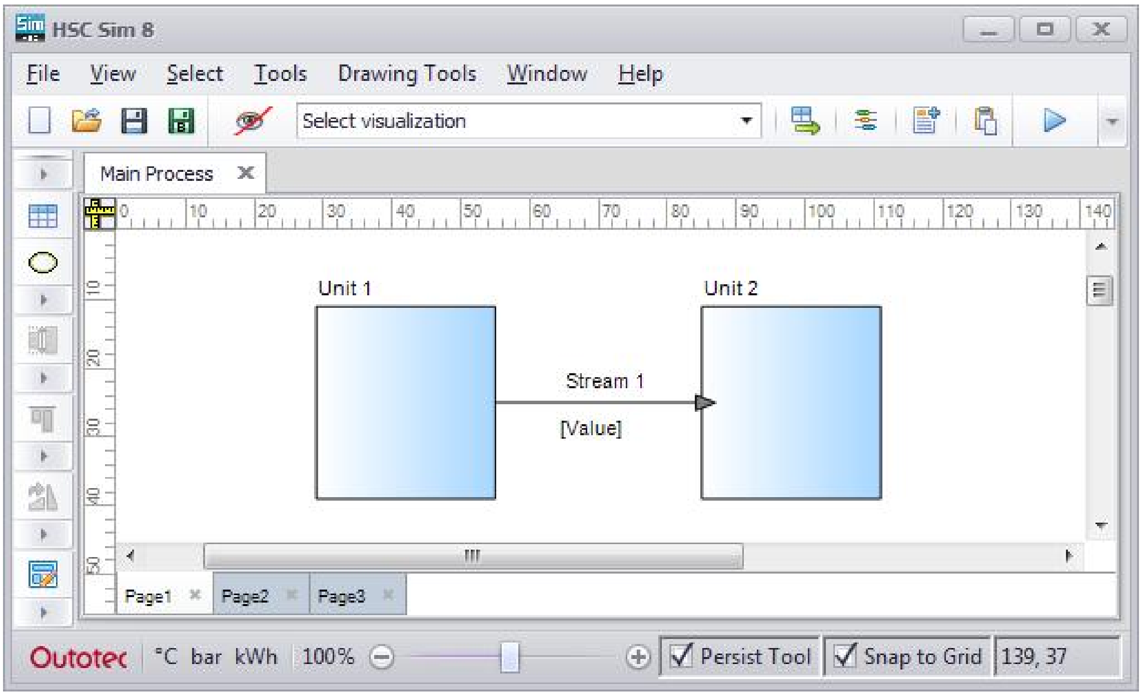


Fig. 9. Adding a unit to a stream between two units, starting situation.

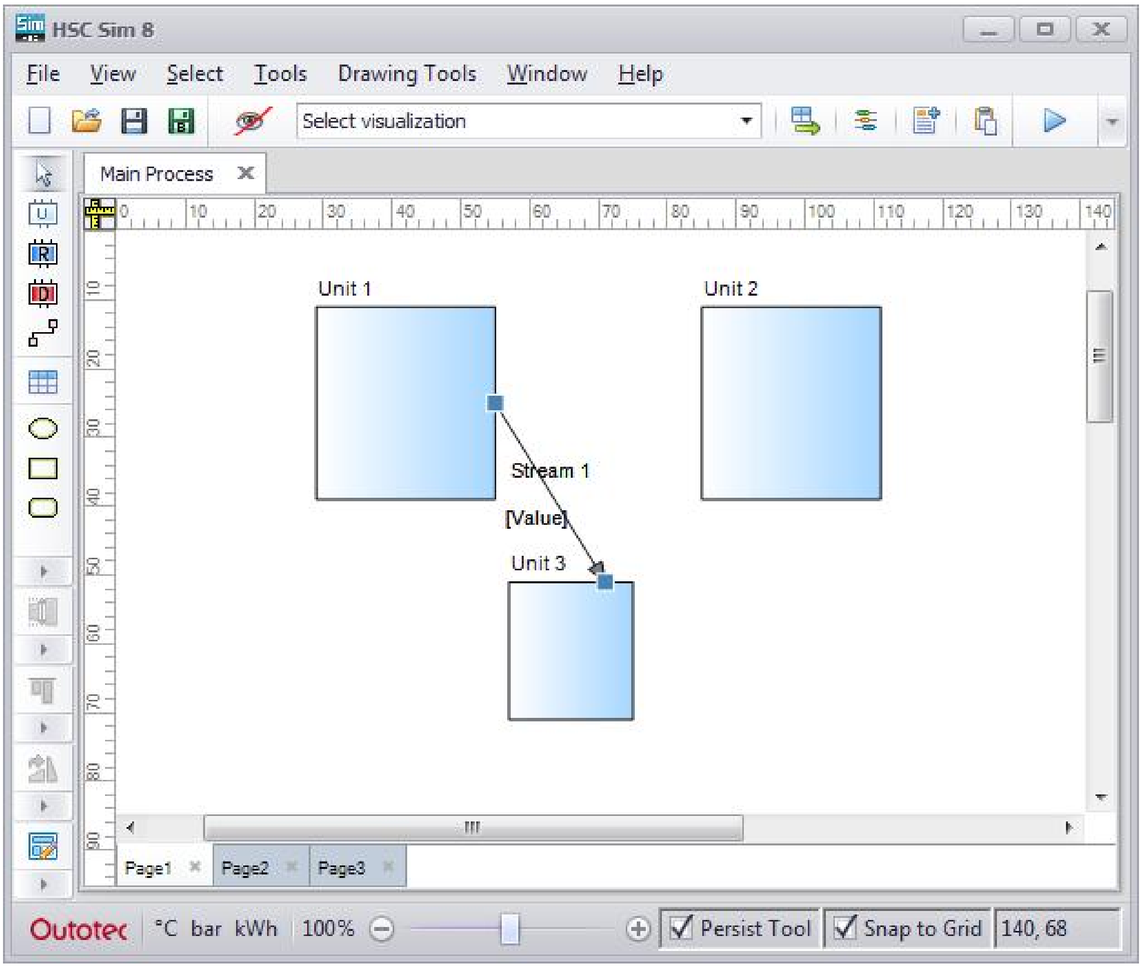


Fig. 10. Adding a unit to a stream between two units, add new unit and change stream connection.

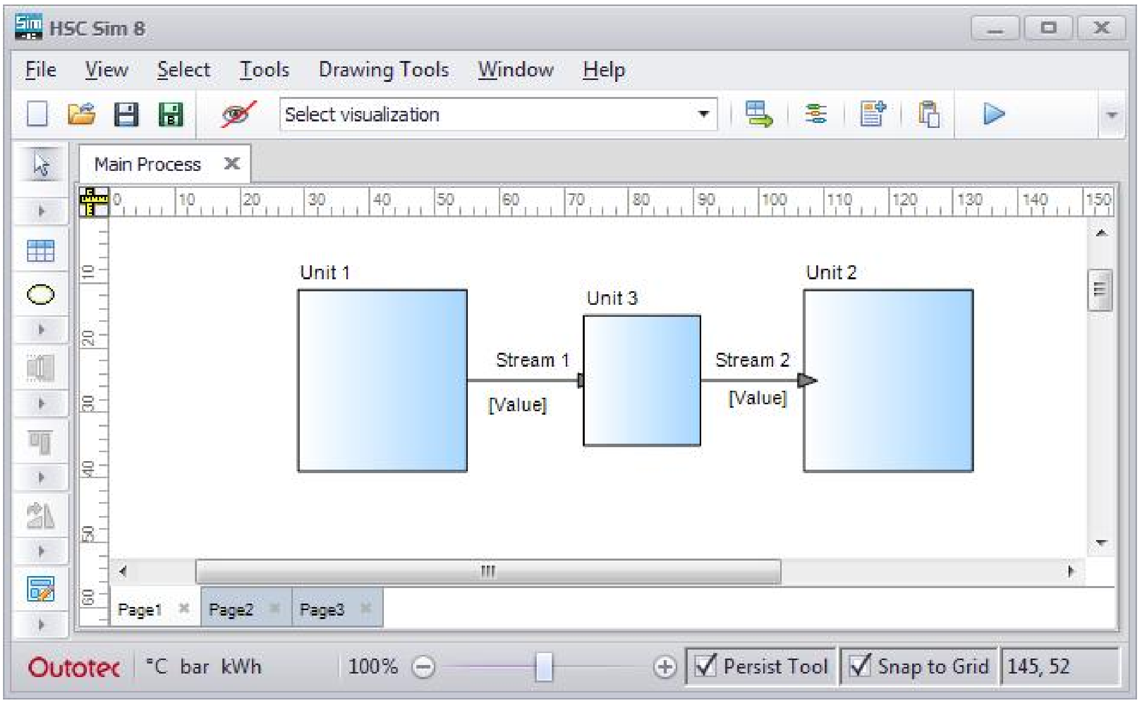


Fig. 11. Adding a unit to a stream between two units, final situation.

40.2. Menus in the flowsheet window

In this section, the Sim flowsheet menus (File, View, Select, Tools, Drawing Tools, Window and Help) are introduced.

File menu

This menu is similar to many other programs where the user can (see also **Fig. 12**):

1. Start **New Process…**which opens an empty flowsheet.
2. **Open Process…**which is a *.Sim8 (HSC8) or *.fls file (HSC7 flowsheet).
3. **Save Process**…quick save process (overwrites previous version)
4. **Save Process as…**save process with the file name and location given by the user
5. **Save Backup…**process should be saved first before a backup can be made. It is recommended to save a backup from time to time during the simulation.
6. **Backups…**If the user has saved backups, they can be managed (checked, restored, deleted) here.
7. **Recent Processes…**shows the 10 most recent simulations made by the user
8. **Export Flowsheet Image…**The user can export the flowsheet as an image (png, vdx, pdf, svg, dxf) or copy a flowsheet picture to the clipboard to use it in reports and presentations.
9. **Print flowsheet…**prints the flowsheet
10. **Exit HSC Sim…**will close the Sim program

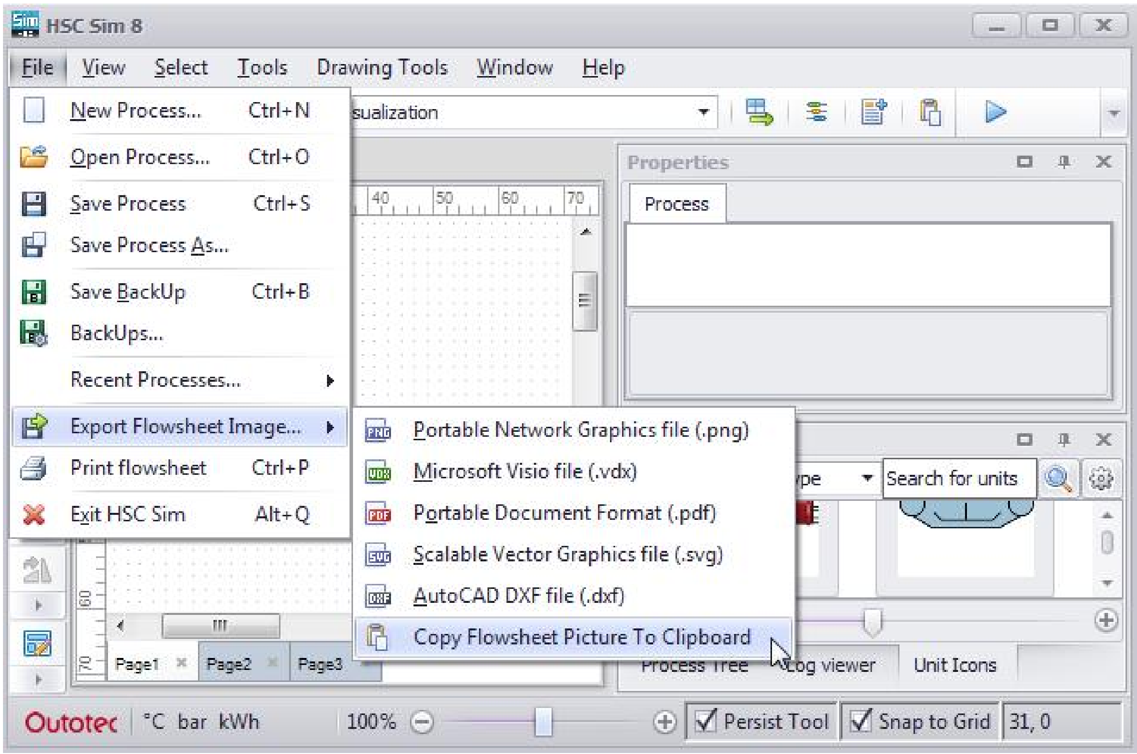


Fig. 12. File menu.

View menu

In the View menu the user can (see also **Fig. 14**):

1. View and edit **Flowsheet settings**, where the user can change or **restore default** settings of the flowsheet. Exit saves the settings and leaves this editor, see **Fig. 13**.

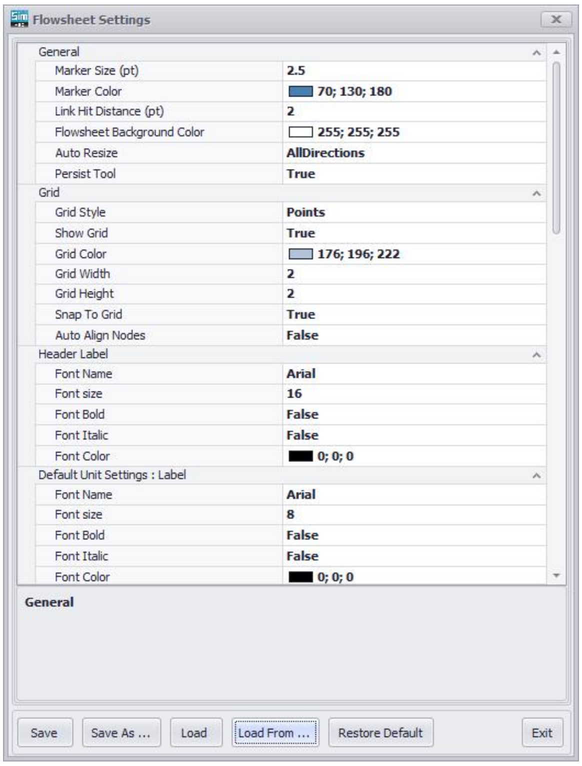


Fig. 13. Flowsheet settings.

2. Show and hide the flowsheet **Name labels, Value labels and Stream tables**.
3. Check and uncheck all **Toolbars**, which are explained in section 40.3.

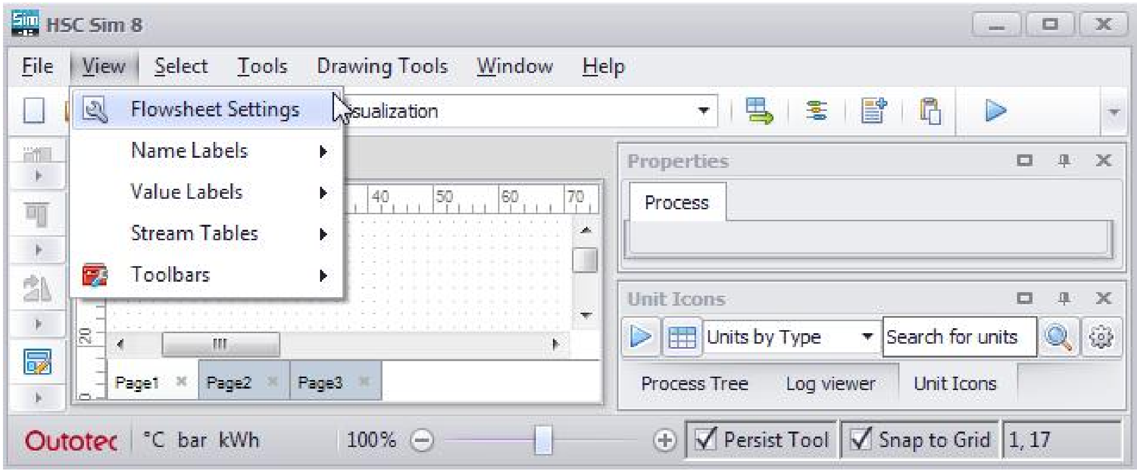


Fig. 14. View menu.

Select menu

The Select menu is typically used to edit or move many properties at once. Here the user can: (see **Fig. 15** below)

1. Select all **Units** on the flowsheet.
2. Select all **Unit Name Labels** on the flowsheet.
3. Select all **Streams** on the flowsheet
4. Select all **Stream Name Labels** on the flowsheet.
5. Select all **Stream Value Labels** on the flowsheet.
6. Select all **Stream Tables** on the flowsheet.
7. Select all (unit and stream) **Name Labels** on the flowsheet.
8. Select all (unit and stream) **Value Labels** on the flowsheet.
9. Select all **Other Text Labels** on the flowsheet.
10. Select **All Labels** on the flowsheet.
11. Select all (not including stream tables) **Tables** on the flowsheet.
12. Select all **Other Drawing Objects** on the flowsheet.
13. Select **All Items** on the flowsheet.

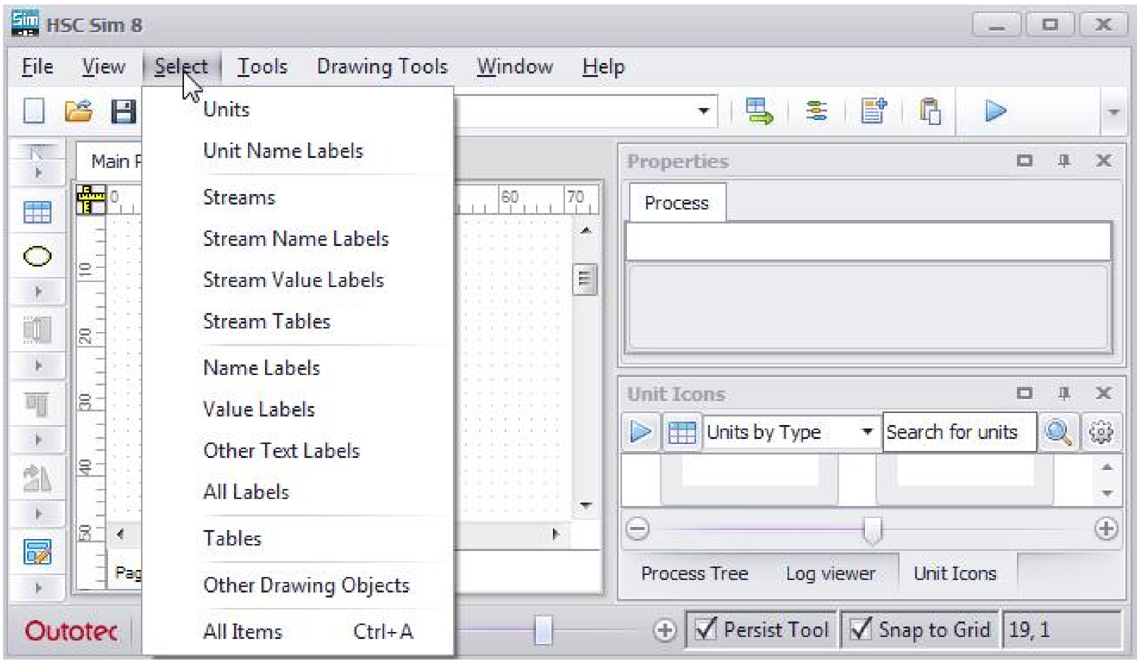


Fig. 15. Select menu.

Tools menu

The Tools menu includes many advanced options that may be needed in flowsheet simulation. The user needs detailed instructions on how to use those tools. Some tools are explained here and others in different Chapters, see the list below. The Tools menu includes (see **Fig. 17**):

1. Process information

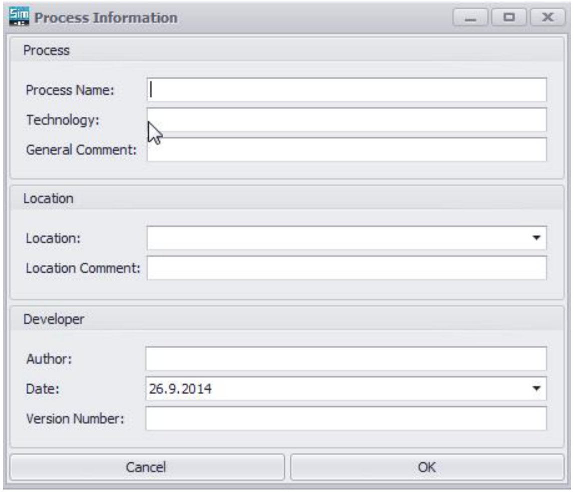


Fig. 16. The user can add Process Information to this sheet.

2. LCA Evaluation (see Chapter 49)
3. Mass Balancing (see Chapters 51 and 52)
4. Reports (see section 40.2.1)
5. Select Unit Models (see section 40.2.2)
6. Scenario Editor (see section 40.2.3)
7. Show the process tree (see section 40.2.4)
8. Errors in flowsheet (shows possible errors in the flowsheet)

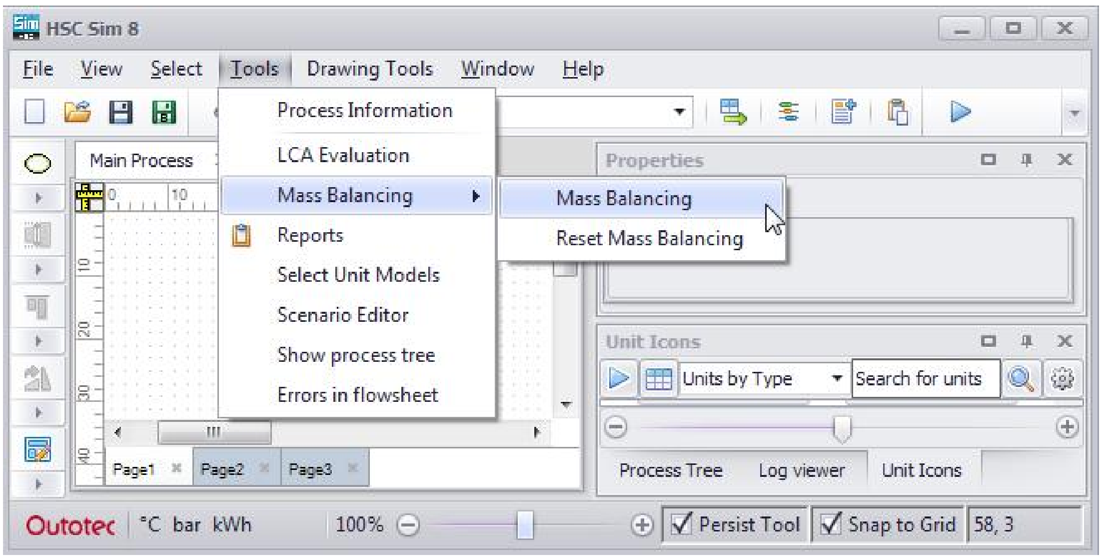
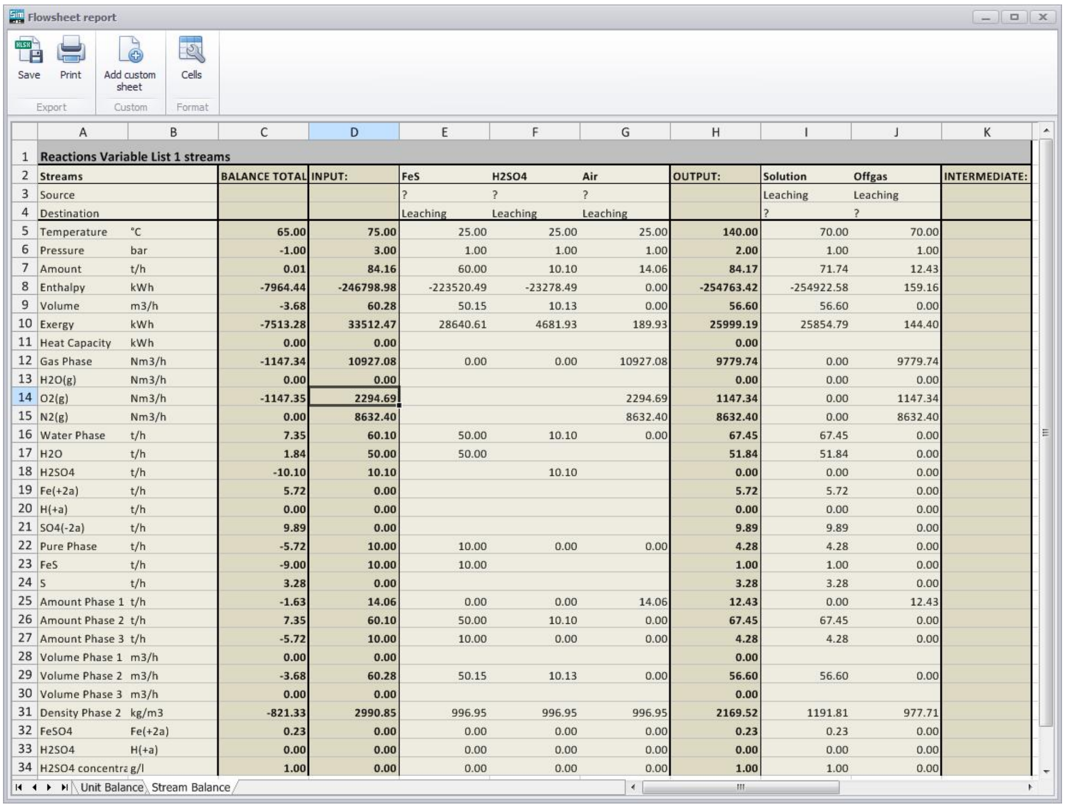


Fig. 17. Tools menu options.

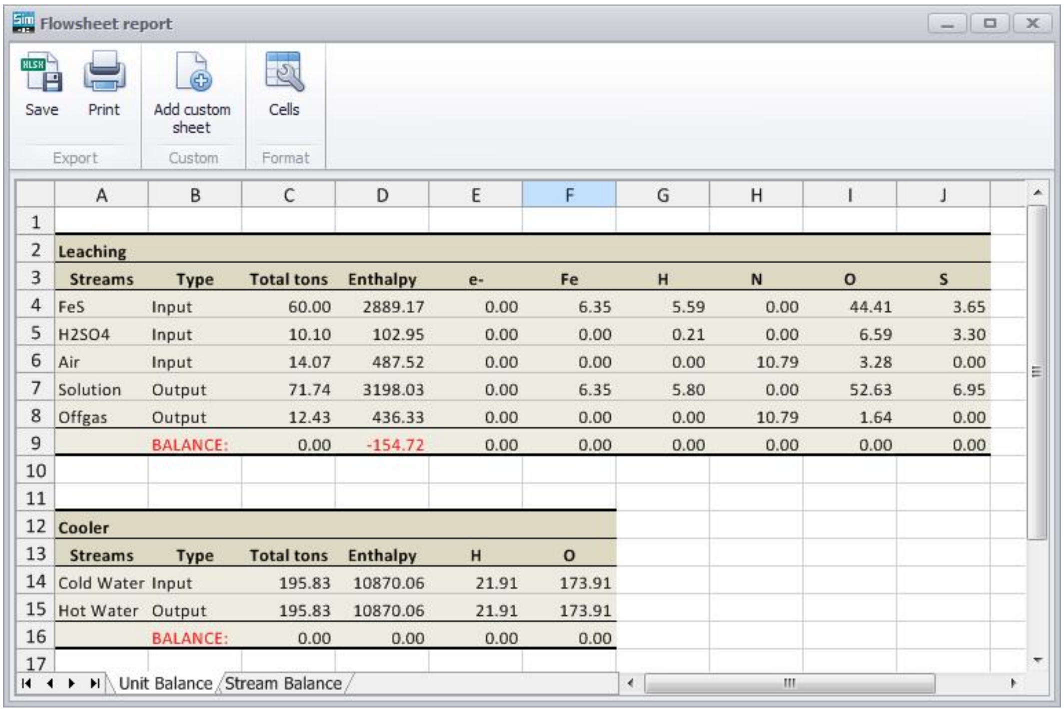
40.2.1. Reports

A summary of flowsheet results can be saved and printed here. There are two pages in this report sheet: one for units and one for streams. This report uses Hydro_example3.Sim8.



	A	B	C	D	E	F	G	H	I	J	K
1	Reactions Variable List 1 streams										
2	Streams		BALANCE TOTAL	INPUT:	FeS	H2SO4	Air	OUTPUT:	Solution	Offgas	INTERMEDIATE:
3	Source				?	?	?		Leaching	Leaching	
4	Destination				Leaching	Leaching	Leaching		?	?	
5	Temperature	°C	65.00	75.00	25.00	25.00	25.00	140.00	70.00	70.00	
6	Pressure	bar	-1.00	3.00	1.00	1.00	1.00	2.00	1.00	1.00	
7	Amount	t/h	0.01	84.16	60.00	10.10	14.06	84.17	71.74	12.43	
8	Enthalpy	kWh	-7964.44	-246798.98	-223520.49	-23278.49	0.00	-254763.42	-254922.58	159.16	
9	Volume	m3/h	-3.68	60.28	50.15	10.13	0.00	56.60	56.60	0.00	
10	Exergy	kWh	-7513.28	33512.47	28640.61	4681.93	189.93	25999.19	25854.79	144.40	
11	Heat Capacity	kWh	0.00	0.00				0.00			
12	Gas Phase	Nm3/h	-1147.34	10927.08	0.00	0.00	10927.08	9779.74	0.00	9779.74	
13	H2O(g)	Nm3/h	0.00	0.00				0.00	0.00	0.00	
14	O2(g)	Nm3/h	-1147.35	2294.69			2294.69	1147.34	0.00	1147.34	
15	N2(g)	Nm3/h	0.00	8632.40			8632.40	8632.40	0.00	8632.40	
16	Water Phase	t/h	7.35	60.10	50.00	10.10	0.00	67.45	67.45	0.00	
17	H2O	t/h	1.84	50.00	50.00			51.84	51.84	0.00	
18	H2SO4	t/h	-10.10	10.10		10.10		0.00	0.00	0.00	
19	Fe(+2a)	t/h	5.72	0.00				5.72	5.72	0.00	
20	H(+a)	t/h	0.00	0.00				0.00	0.00	0.00	
21	SO4(-2a)	t/h	9.89	0.00				9.89	9.89	0.00	
22	Pure Phase	t/h	-5.72	10.00	10.00	0.00	0.00	4.28	4.28	0.00	
23	FeS	t/h	-9.00	10.00	10.00			1.00	1.00	0.00	
24	S	t/h	3.28	0.00				3.28	3.28	0.00	
25	Amount Phase 1	t/h	-1.63	14.06	0.00	0.00	14.06	12.43	0.00	12.43	
26	Amount Phase 2	t/h	7.35	60.10	50.00	10.10	0.00	67.45	67.45	0.00	
27	Amount Phase 3	t/h	-5.72	10.00	10.00	0.00	0.00	4.28	4.28	0.00	
28	Volume Phase 1	m3/h	0.00	0.00				0.00			
29	Volume Phase 2	m3/h	-3.68	60.28	50.15	10.13	0.00	56.60	56.60	0.00	
30	Volume Phase 3	m3/h	0.00	0.00				0.00			
31	Density Phase 2	kg/m3	-821.33	2990.85	996.95	996.95	996.95	2169.52	1191.81	977.71	
32	FeSO4	Fe(+2a)	0.23	0.00	0.00	0.00	0.00	0.23	0.23	0.00	
33	H2SO4	H(+a)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
34	H2SO4 concentra	g/l	1.00	0.00	0.00	0.00	0.00	1.00	1.00	0.00	

Fig. 18. Stream balance sheet of the report file.



	A	B	C	D	E	F	G	H	I	J
1										
2	Leaching									
3	Streams	Type	Total tons	Enthalpy	e-	Fe	H	N	O	S
4	FeS	Input	60.00	2889.17	0.00	6.35	5.59	0.00	44.41	3.65
5	H2SO4	Input	10.10	102.95	0.00	0.00	0.21	0.00	6.59	3.30
6	Air	Input	14.07	487.52	0.00	0.00	0.00	10.79	3.28	0.00
7	Solution	Output	71.74	3198.03	0.00	6.35	5.80	0.00	52.63	6.95
8	Offgas	Output	12.43	436.33	0.00	0.00	0.00	10.79	1.64	0.00
9		BALANCE:	0.00	-154.72	0.00	0.00	0.00	0.00	0.00	0.00
10										
11										
12	Cooler									
13	Streams	Type	Total tons	Enthalpy	H	O				
14	Cold Water	Input	195.83	10870.06	21.91	173.91				
15	Hot Water	Output	195.83	10870.06	21.91	173.91				
16		BALANCE:	0.00	0.00	0.00	0.00				
17										

Fig. 19. Unit balance sheet of the report file.

40.2.2. Select Unit Models

The user can choose different models for the units. The Select Unit Models window can be opened from the Tools menu or by right-clicking if the cursor is on top of one of the units, see **Fig. 20**. On the left side of the window is the list of units on the flowsheet. In the middle part the user can select a unit model from the Reactions, Distribution, Particle and Others sheet (and in the HSC8 update also 'Import own unit models'). **Double-click** the unit to select it and then click OK. Most of the units are dll type but there are still some Excel Wizards available for the Reactions units. If Excel Wizards are chosen, the user needs to check the stream names. Information about the units can be found on the right side of the selector window. Empty Reactions or Distributions units are the same as R and D unit Icons on the main flowsheet DrawBar, see **Fig. 1**.

In the HSC8 update that comes later, there will be instructions on how users can make their own dll units (Chapter 50). User-made units can be imported using the import sheet.

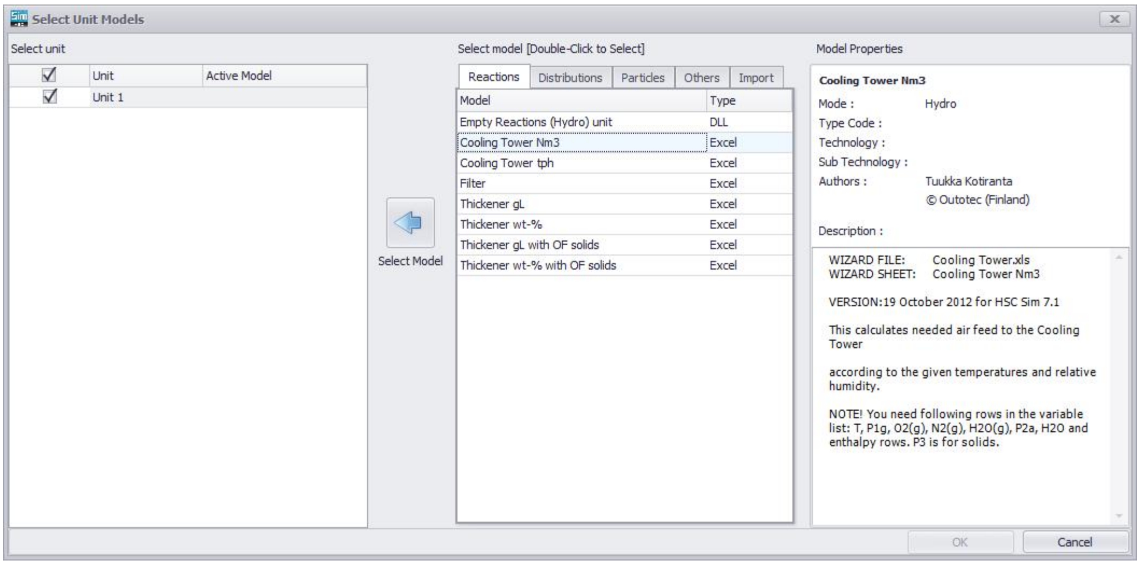


Fig. 20. Select Unit Models window.

40.2.3. Scenario Editor

The Scenario Editor lets you run your process model with different operating parameters and see how they affect process variables. The calculated results can then be collected in the charts.

To use the Scenario Editor, first select the processing parameter that you want to regulate and copy its cell reference from the appropriate cell. Next, open the Scenario Editor and paste the cell reference in the first SET/GET column (**Fig. 21**). Then you can add a name and measurement unit for this variable, but most importantly you should specify whether the variable will be a regulated (SET) or a calculated variable (GET) (**Fig. 22**).

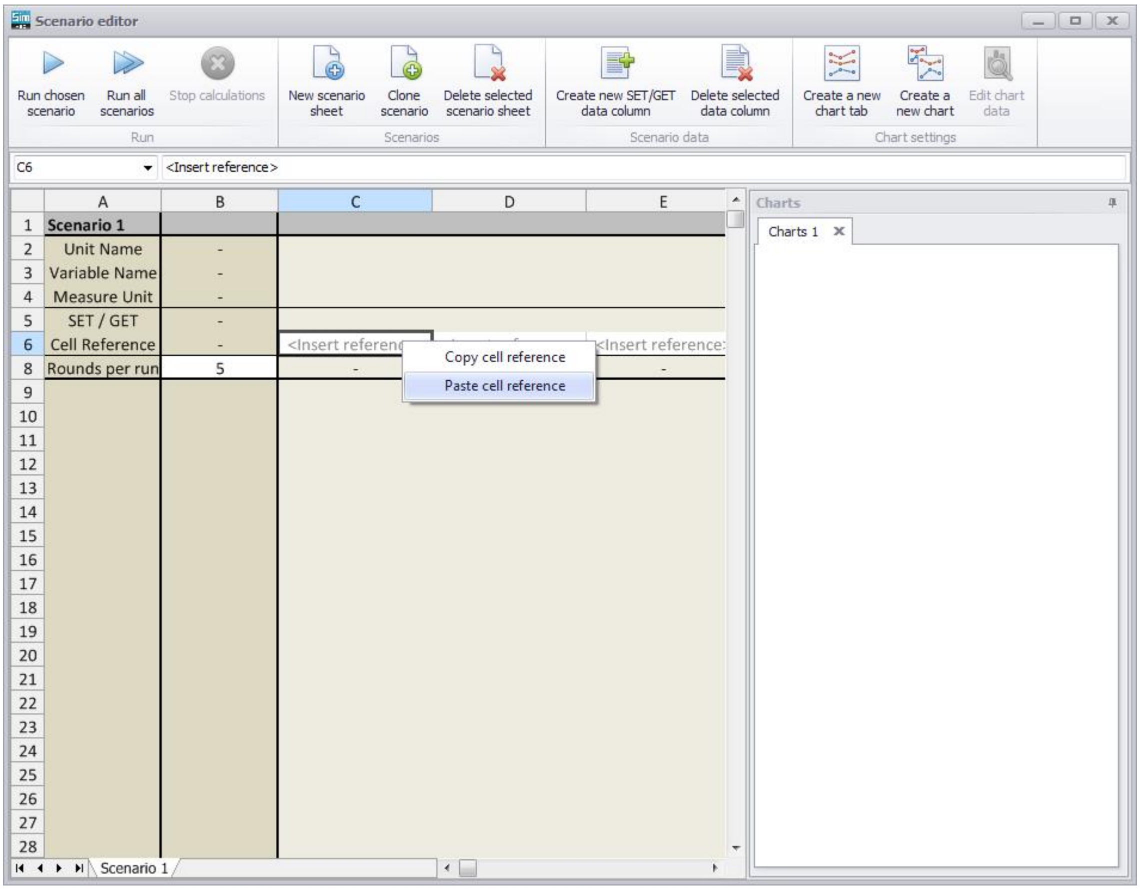


Fig. 21. Add variables to the Scenario Editor by pasting the cell reference of the variable cell.

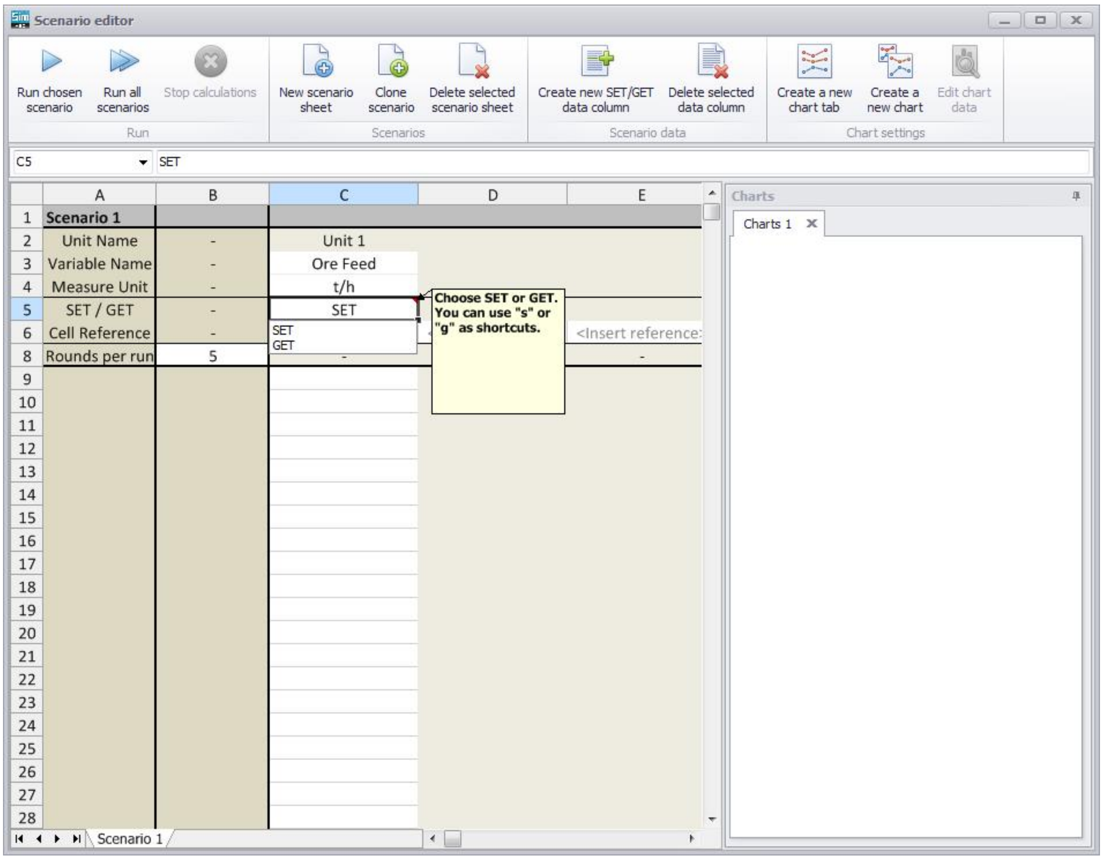


Fig. 22. Specify the SET/GET value for the variable.

After adding enough variables, specify the parameter values for the SET columns, add some charts, and finally run the scenario (**Fig. 23**).

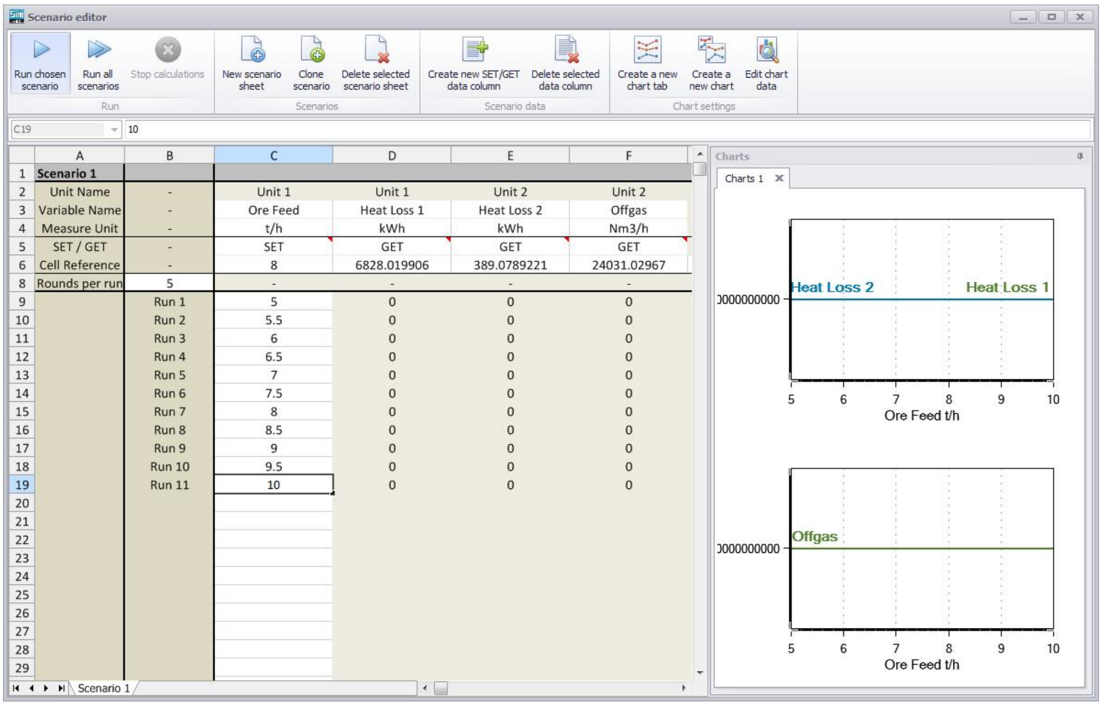
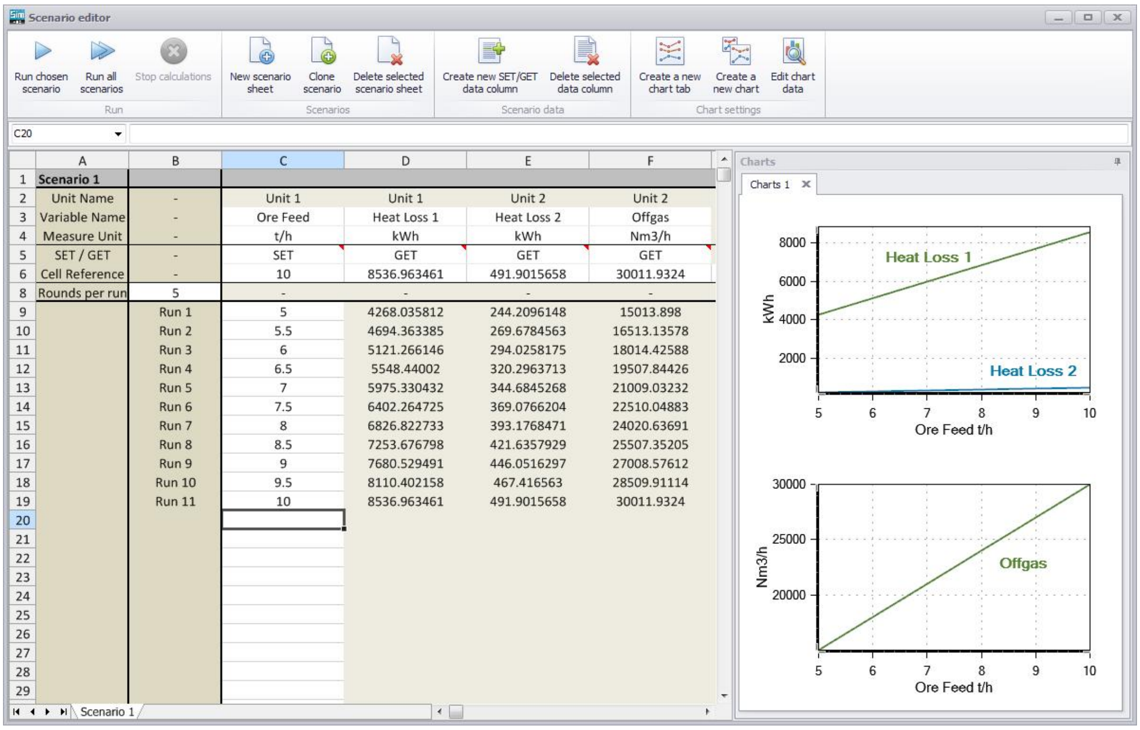


Fig. 23. After specifying the variables, enter the SET variable values, add charts, and run the scenario.

The calculation results will then be presented in the spreadsheet as well as in the charts (**Fig. 24**).



	A	B	C	D	E	F
1	Scenario 1					
2	Unit Name	-	Unit 1	Unit 1	Unit 2	Unit 2
3	Variable Name	-	Ore Feed	Heat Loss 1	Heat Loss 2	Offgas
4	Measure Unit	-	t/h	kWh	kWh	Nm3/h
5	SET / GET	-	SET	GET	GET	GET
6	Cell Reference	-	10	8536.963461	491.9015658	30011.9324
8	Rounds per run	5	-	-	-	-
9		Run 1	5	4268.035812	244.2096148	15013.898
10		Run 2	5.5	4694.363385	269.6784563	16513.13578
11		Run 3	6	5121.266146	294.0258175	18014.42588
12		Run 4	6.5	5548.44002	320.2963713	19507.84426
13		Run 5	7	5975.330432	344.6845268	21009.03232
14		Run 6	7.5	6402.264725	369.0766204	22510.04883
15		Run 7	8	6826.822733	393.1768471	24020.63691
16		Run 8	8.5	7253.676798	421.6357929	25507.35205
17		Run 9	9	7680.529491	446.0516297	27008.57612
18		Run 10	9.5	8110.402158	467.416563	28509.91114
19		Run 11	10	8536.963461	491.9015658	30011.9324

Fig. 24. Results of the scenario.

40.2.4. Show Process Tree

With this option the user can see the flowsheet information and connections of the process streams with colors. If a stream is not connected to the unit, it will not be visible in this process tree.

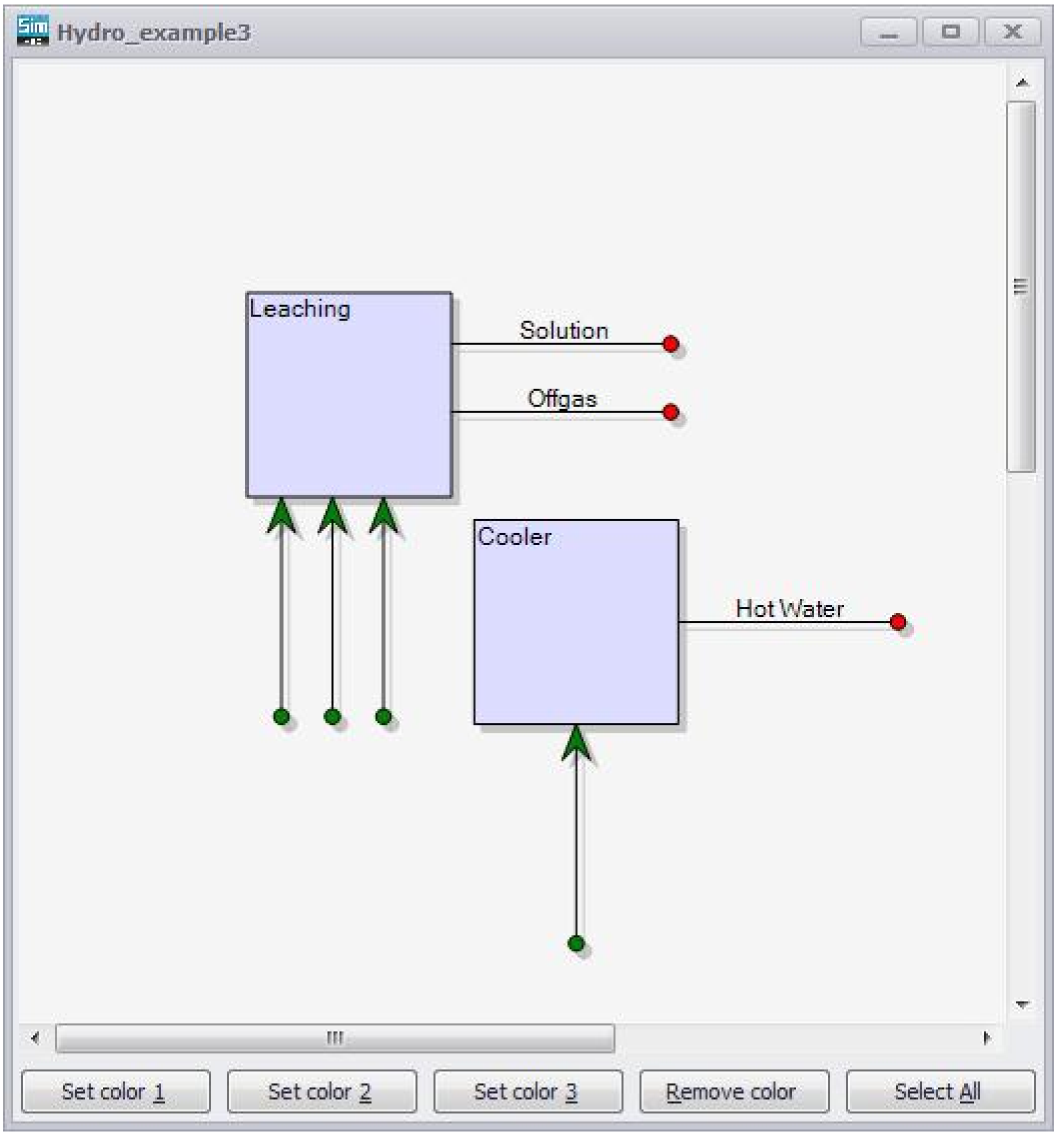


Fig. 25. Show process tree.

Drawing Tools menu

The user can edit the flowsheet using Drawing Tools by aligning, sizing, rotating, grouping, and drawing, see **Fig. 26**.

One handy way of editing the flowsheet is Edit Pages and Layers where you can set layers and properties which are visible or invisible on your flowsheet, see **Fig. 27**.

The user can find more details about Drawing Tools in section 40.3.

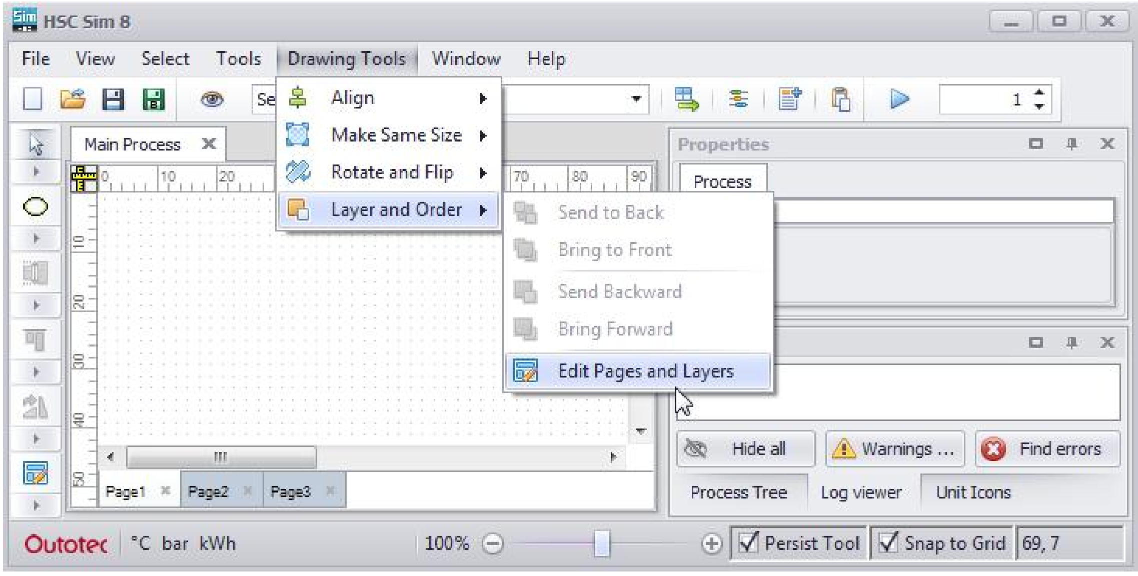


Fig. 26. Drawing tools.

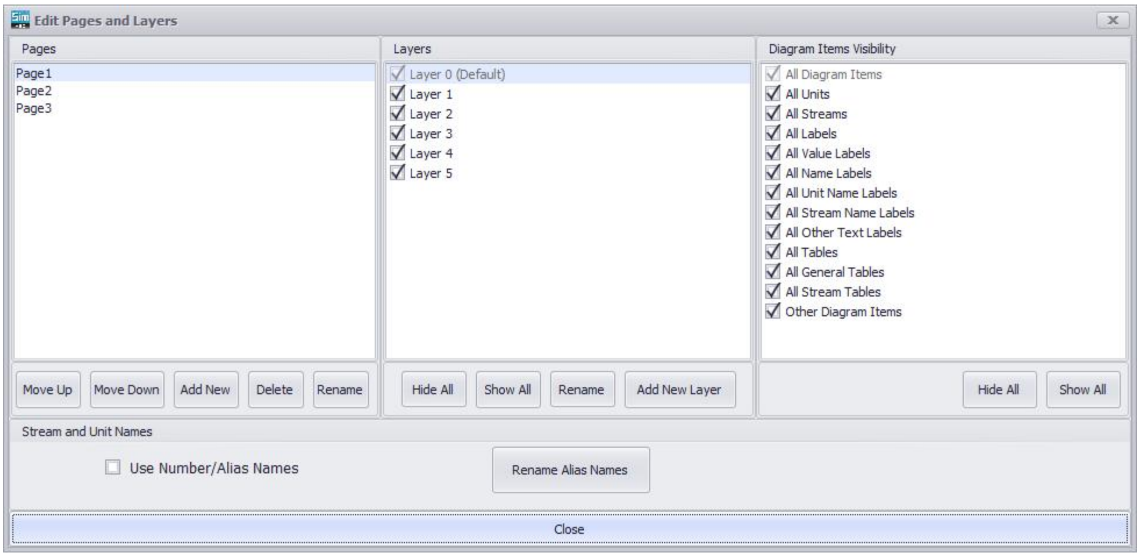


Fig. 27. Edit Pages and Layers window.

Window and Help menus

The Window menu shows the user the name of the flowsheet, see **Fig. 28**.

The Help menu shows a list of software developers and technical advisors and a link to the Sim manual, see **Fig. 29** and **Fig. 30**.

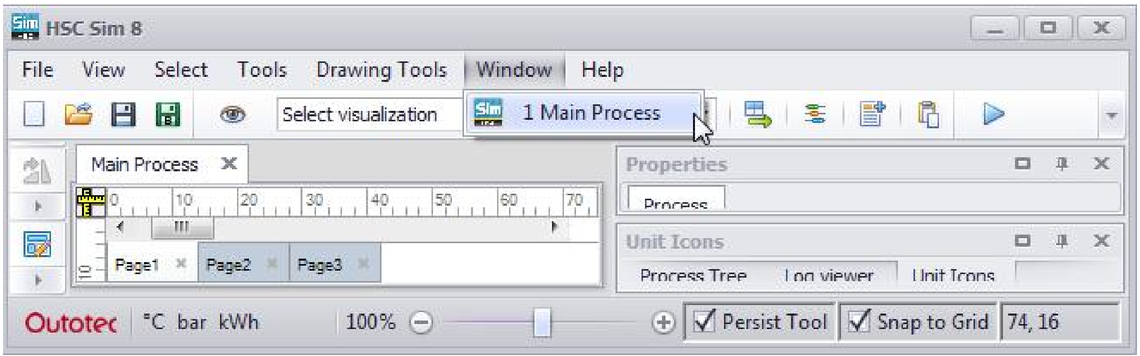


Fig. 28. Window menu.

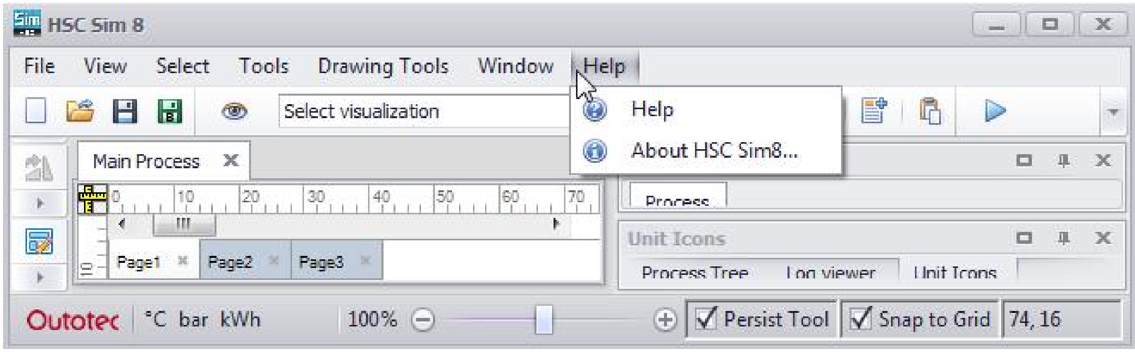


Fig. 29. Help menu.

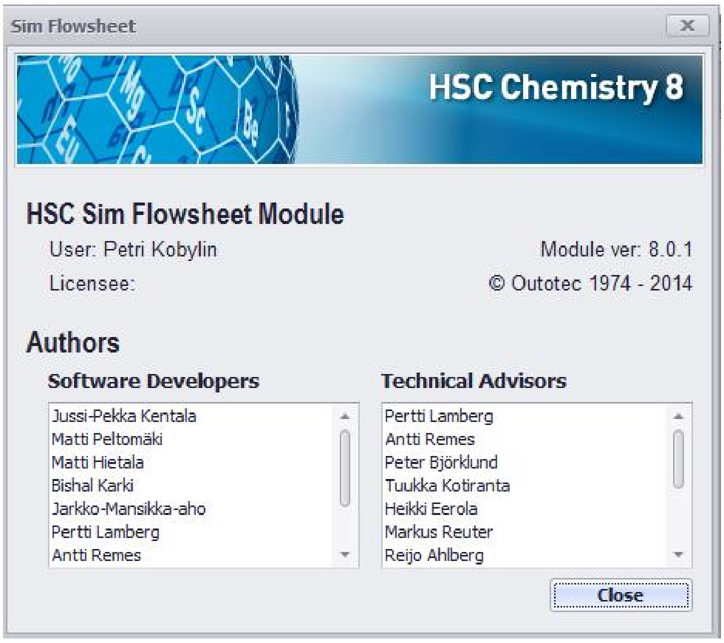


Fig. 30. About HSC8 Sim.

40.3. Toolbars

In the View Toolbars menu, the user can check and uncheck toolbars. It is also possible to reset docking bar positions back to their default places. Toolbars are divided into two lists: Docking bars and Drawing toolbars, see **Fig. 31**.

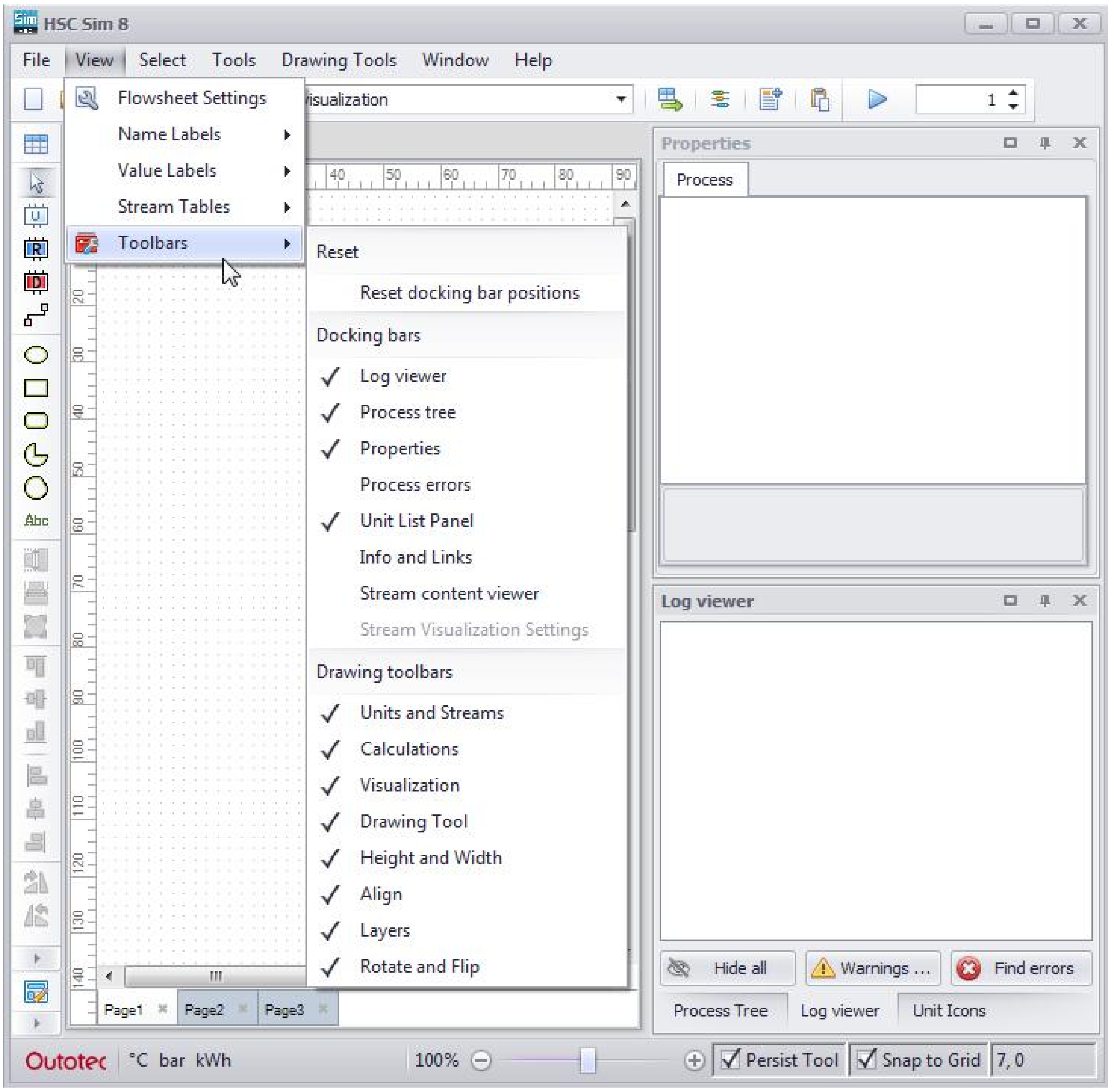


Fig. 31. List of toolbars.

40.3.1. Drawing toolbars

The Drawing toolbars are listed and guidance on their usage briefly described in **Fig. 32** - **Fig. 42**. Many drawing options can be later edited from docking toolbar **Properties** after they have been drawn (section 40.3.2).

Fig. 32. Units and streams. Select or Draw Units or Draw Streams (see also section 40.1).

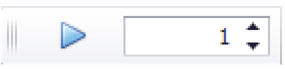


Fig. 33. Calculations. Simulate and give iteration rounds for calculations.

Fig. 34. Visualization. Select or unselect visualization mode and select the stream property that is visualized. The user can also change measurement units, open the Stream Table Editor, visualize stream connections, add a header and copy the flowsheet picture to the clipboard using this toolbar.

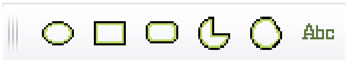


Fig. 35. Drawing tool. With this toolbar the user can add shapes like an ellipse, rectangle, rounded rectangle, pie and chord. It is also possible to add a textbox.

Fig. 36. Height and Width. With this toolbar the user can make the size of the selected units or streams equal.

Fig. 37. Align. With this toolbar the user can align selected units in many ways, thus making it easier to draw professional-looking flowsheets.

Fig. 38. Layers. With this toolbar the user can edit pages and layers (**Fig. 27**) or change the position of overlapping units.

Fig. 39. Rotate and Flip. With this toolbar the user can rotate or flip units.

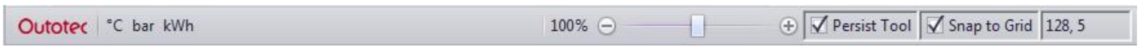


Fig. 40. Status bar. With the status bar the user can zoom the flowsheet and check and uncheck the Persist Tool and Snap to Grid options. The **Persist Tool** remembers the last used drawing tool so that the user does not have to select the same tool again separately. The **Snap to Grid** option aligns the streams and units according to the grid on the flowsheet, thus making it easier to draw professional-looking flowsheets.

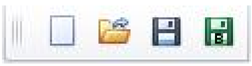


Fig. 41. FileBar. The user can start a new, open an old, save the current process and save a backup of the current process using this toolbar.

Fig. 42. TableBar. The user can insert a table using this toolbar (see also section 40.1.4).

40.3.2. Docking bars

Fig. 43. Log viewer. This docking bar shows the user possible warnings and errors found during the simulation.

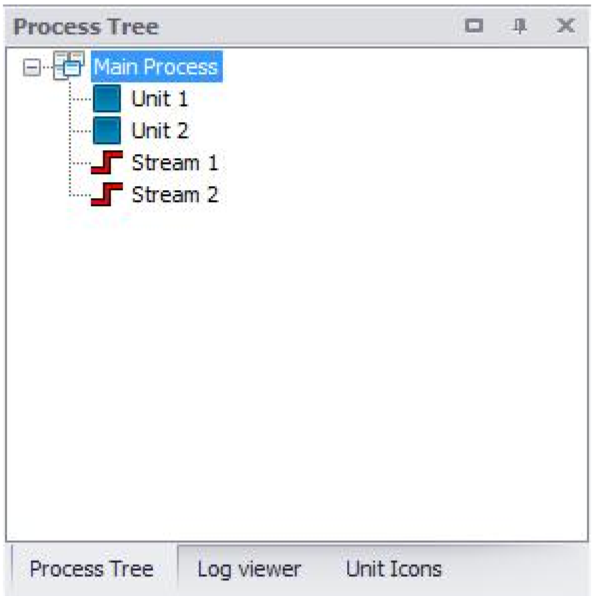


Fig. 44. Process Tree. In this docking bar the user sees the flowsheet as a process tree.

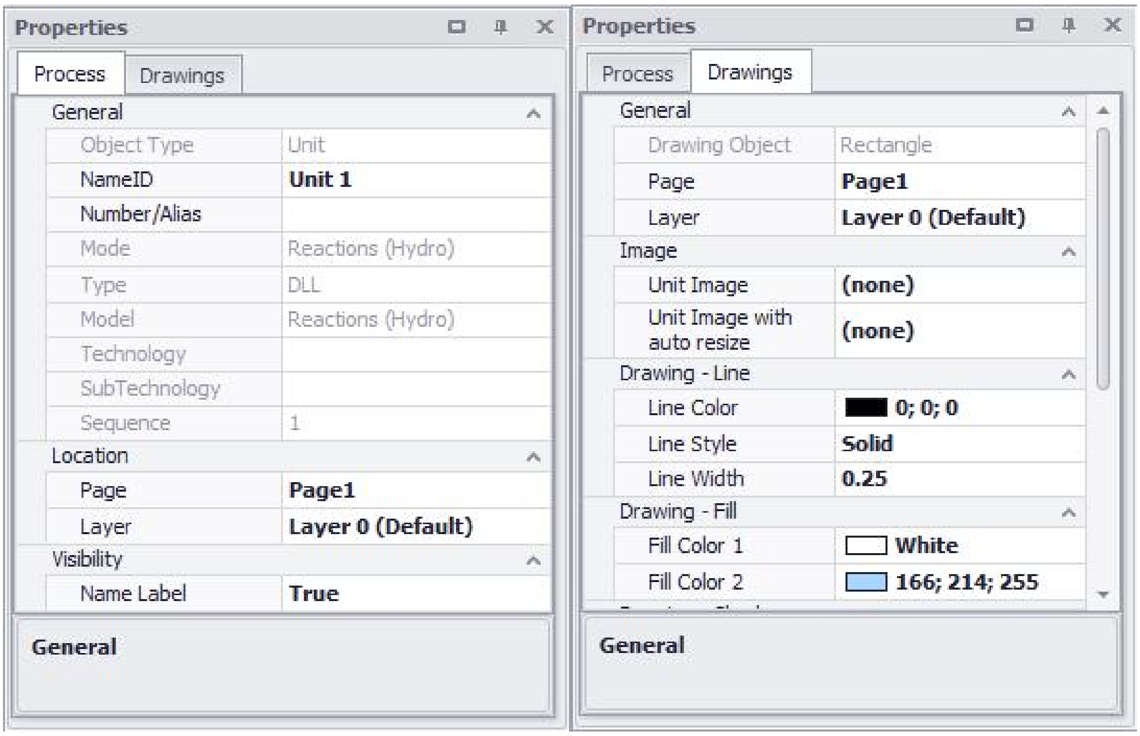


Fig. 45. Properties - **Unit** Process and Drawings.

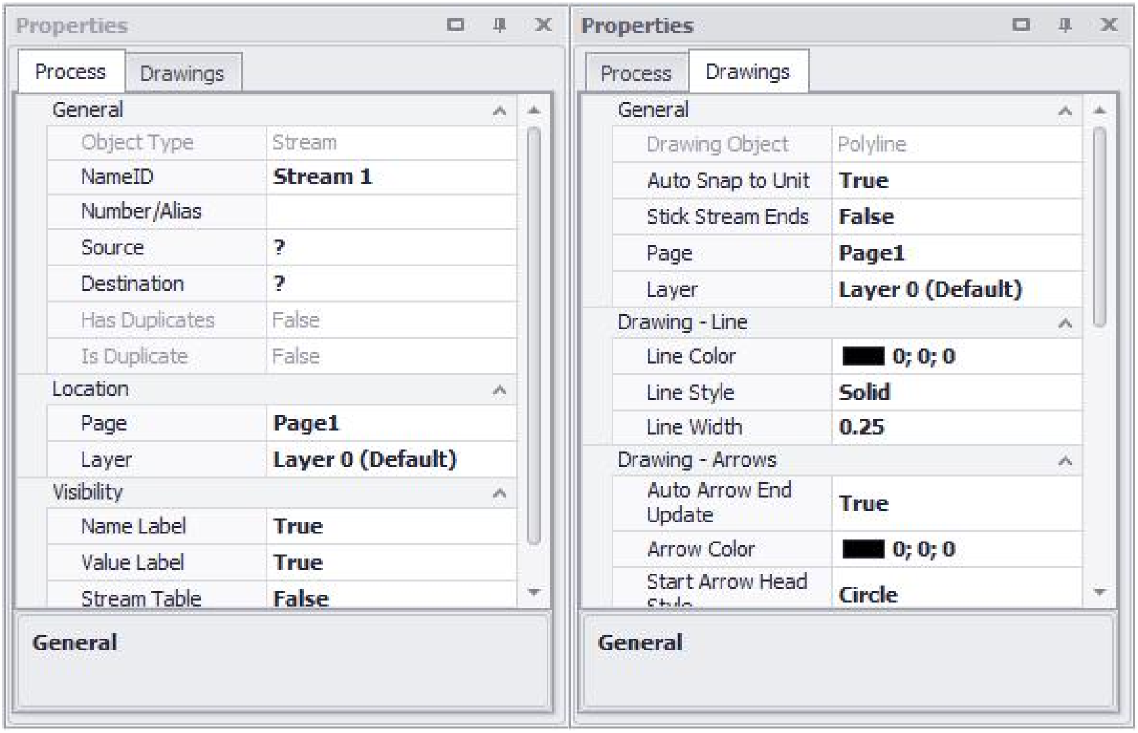


Fig. 46. Properties - **Stream** Process and Drawings.

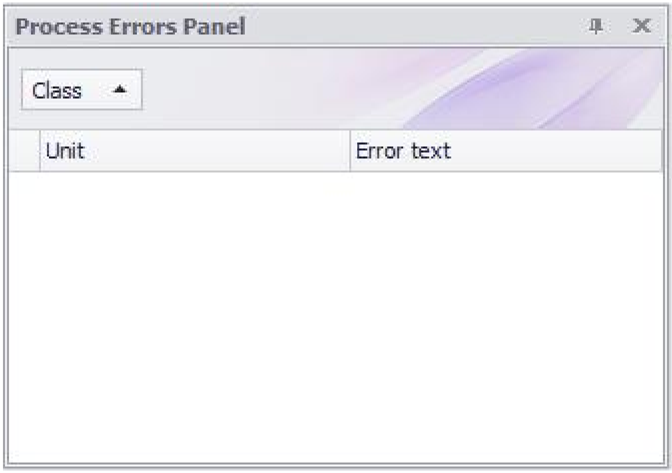


Fig. 47. Process Errors.

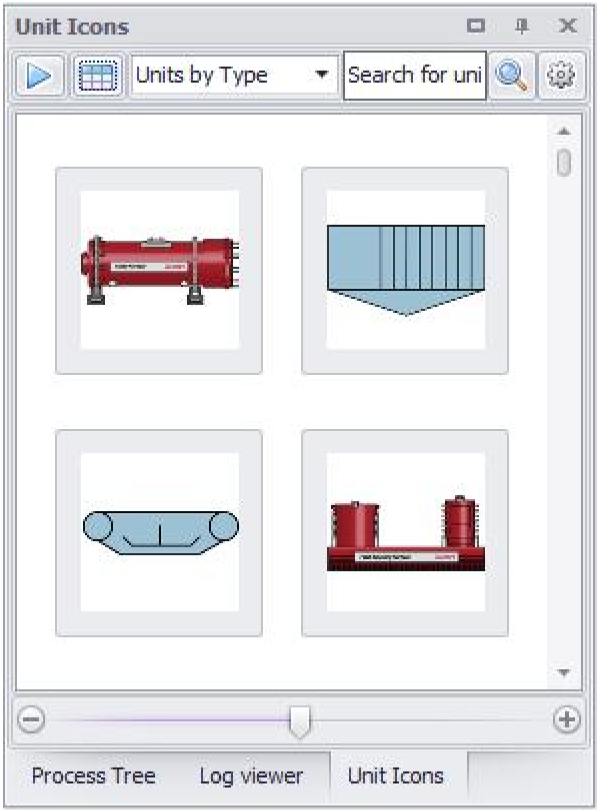


Fig. 48. Unit Icons (Unit List Panel). With this docking bar the user can add Unit pictures to the flowsheet. The unit pictures are of generic type (see section 40.2.2). The user can switch the view, browse picture location, search by name, or change unit directory (top bar) or zoom icons (bottom bar).

Fig. 49. Info and Links. The user can add for example instructions on how to use the flowsheet here.

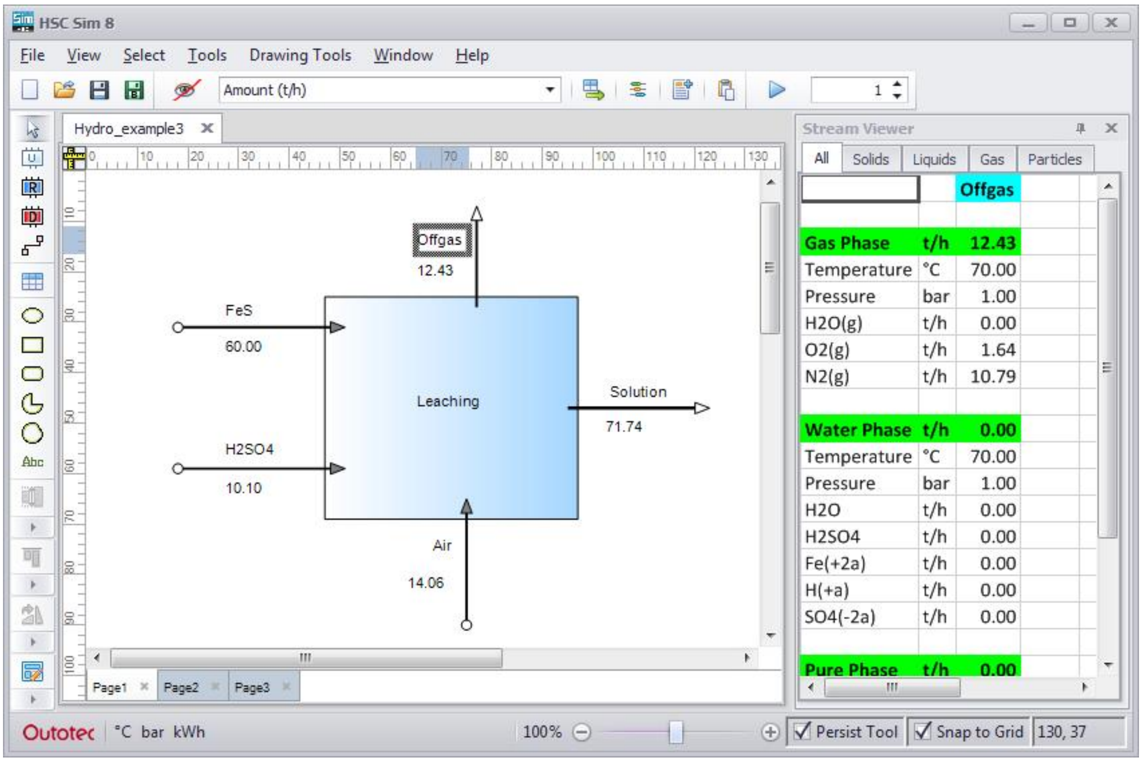


Fig. 50. Stream Content Viewer. In this docking bar the user can see a tabulated summary of the stream properties.

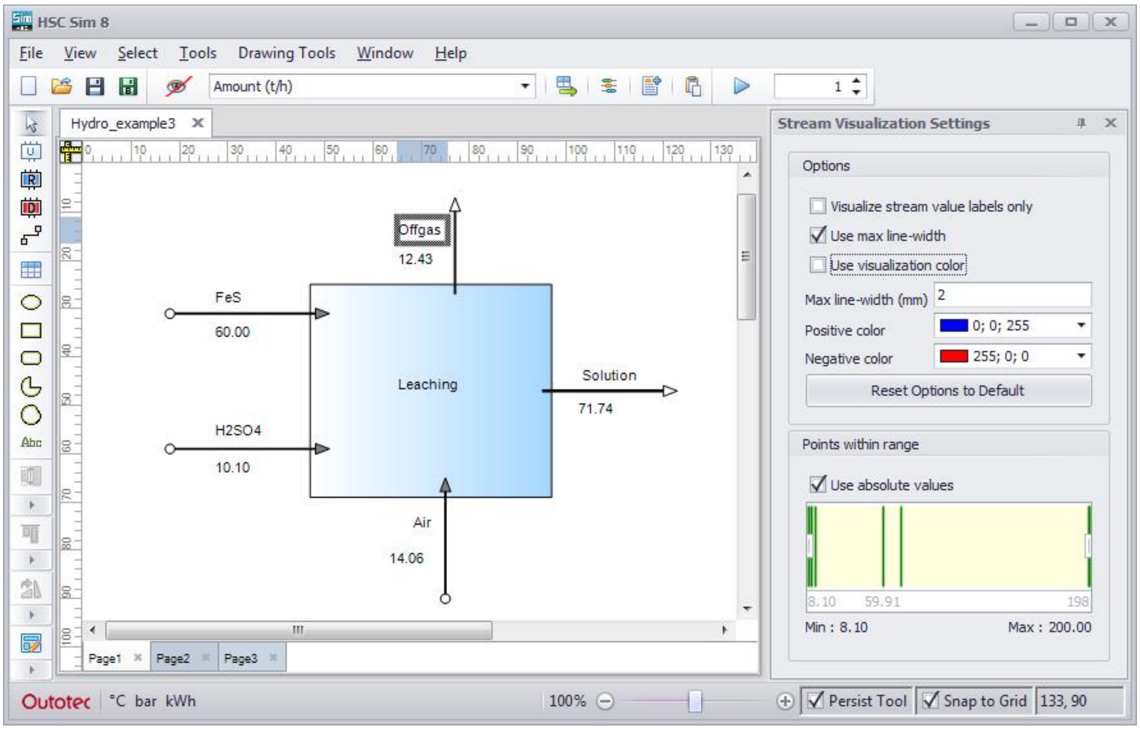


Fig. 51. Stream Visualization Settings. In this docking bar the user can change the settings of the Sankey diagram (thickness of the stream shows where most of the material goes).

40.4. Importing HSC Sim 7 models (HSC Sim 6 models are not supported)

In HSC Sim 8 there is a built-in support for importing HSC Sim 7 models and then using them in Sim 8. However, there are some points and limitations that the user should take into consideration when importing Sim 7 models into Sim 8. If points listed here do not help please contact the developers.

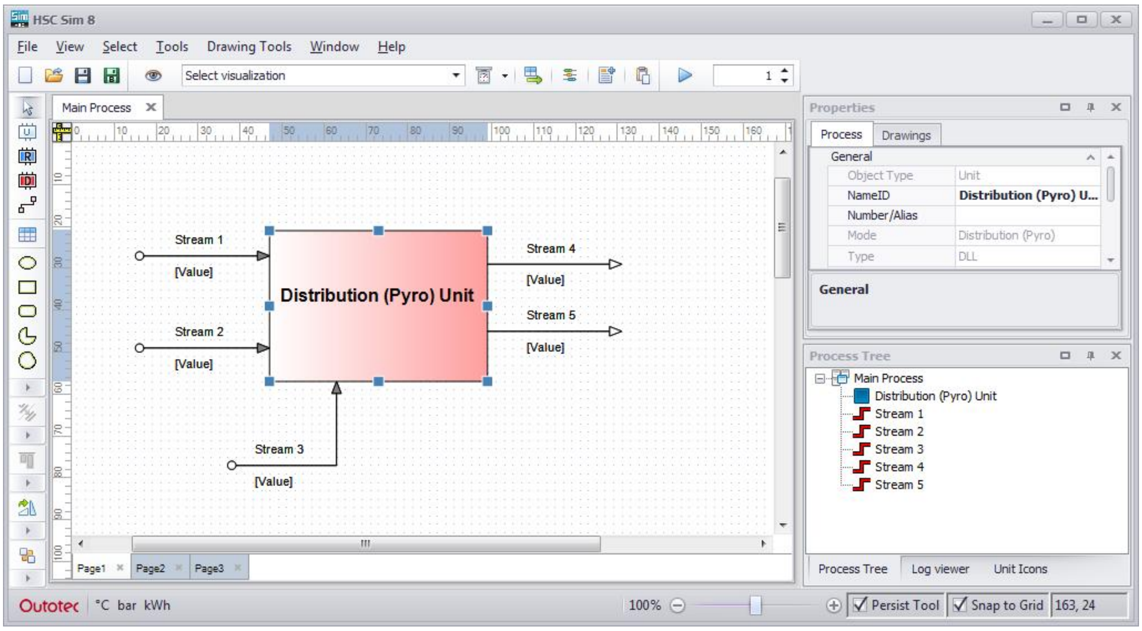
Major points:

- Sim 8 calculations have dramatically stricter error checks than Sim 7. When the user imports an old model and tries to run it, often the calculation will notify of an error in the flowsheet. The user can locate the errors using the log viewer and then fix them manually.
- There are some changes in the Sim 8 hydro variable list logic when compared to Sim 7. If the imported model variable list contains species not found in the database, the user needs to go through them case by case in the Sim 8 variable list editor. The user can add entries to the database, use a different database entry, or delete the species from the variable list to fix this (see Chapter 43, section 43.2.1).
- Sim 7 solvent extraction hydro Excel Wizards are no longer supported in Sim 8. If the imported model contains them in Sim 8, the user will not be able to run the model successfully.
- There is a completely new DLL unit operation system in Sim 8, which has been implemented for some Mineral Process unit operation models. Sim 8 has partial support for using old Sim 7 minpro Excel Wizard models and the user should be able to run calculations for the imported Sim 7 minpro Excel Wizards. However, the user cannot currently edit or make the Excel Wizards for the old minpro models. If users want to edit their old mineral process models, they should replace the old minpro Excel Wizards with the new DLL models.

Minor points:

- Sim 8 uses different Stream Tables than Sim 7. Because of this, users cannot edit Sim 7 Stream Tables in Sim 8 but they can make new ones using Sim 8 tools.
- The visibility of the connected streams is forced on for input and output streams in Sim 8. If there are any such streams hidden in the imported Sim 7 model, they will appear in Sim 8.
- A few drawing objects like a Bézier curve are not supported in the first version of Sim 8.
- In some rare cases, Sim 8 does not recognize Sim 7 stream connections correctly. Information about this will be given in the import log. Afterwards the user should manually confirm the notified stream connections.
- In Sim 7, the user had the possibility to encrypt some units. This function is no longer supported in Sim 8, which means those units will not be loaded during the import.
- External workbook references work differently in Sim 7 and Sim 8. When you import a Sim 7 model, all external references are changed and will include “REF” at the beginning of the reference.
- Sim 7 used automatically safe division for all division operations in the workbook. This meant that, for example, 0/0 did not give an error as the answer. Sim 8 adds the “safediv” function to division operations.
- Sim 8 will change the sheet names of the workbook if the sheet contains illegal characters like “/”.

41. Sim Distribution (Pyro) Units



The Distribution unit, also known as the Pyro unit, is a basic unit type in which output species are formed based on the element distribution. This distribution can be defined manually, and regulated further with controls. The Distribution unit also offers Mixer and Equilibrium wizards which allow you to produce the output species without defining the element distribution.

41.1. Steps to Successful Sim Distribution Simulation

It is important to add the necessary information before simulation can be started. It is good to follow this list while making your Sim Distribution models. Steps 2 to 5 are explained in more detail here.

1. Draw units and streams
2. Specify input streams
3. Specify output streams
4. Specify distribution
5. Set controls
6. Save process
7. Run process

41.2. Specify Input Streams

The unit editor for a distribution unit is shown in **Fig. 1**. Information about the input streams is specified on the Input sheet. The data of the streams are presented in rows. For the input streams, you should specify: the total amount of the stream, the measurement unit for the total amount, temperature, pressure, species, and composition.

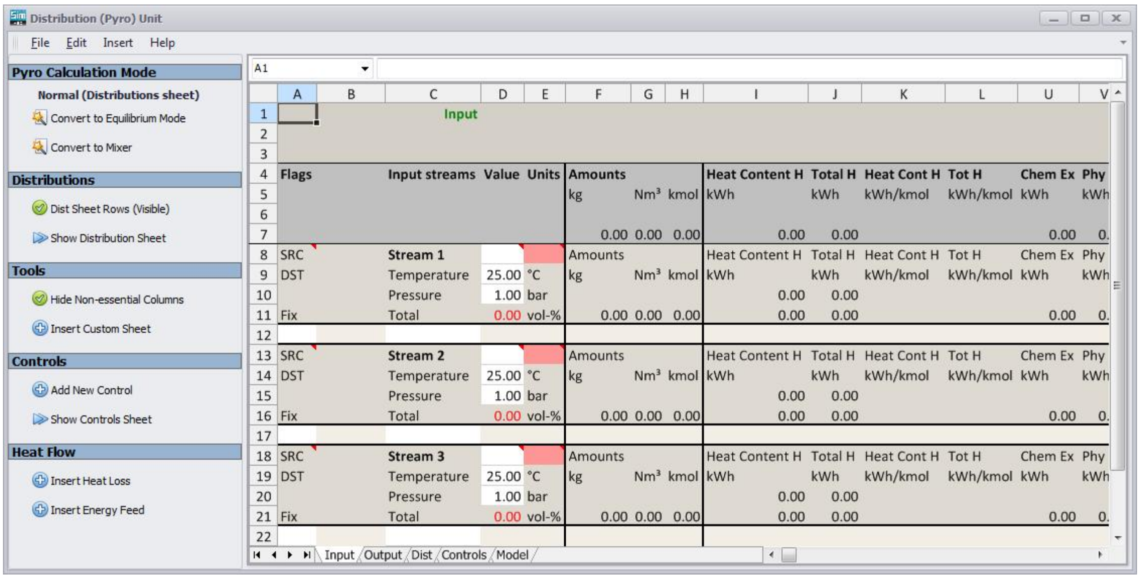


Fig. 1. Distribution unit editor.

41.2.1. Total Amount, Temperature and Pressure

The total amount of the input stream is specified in the cell next to the stream name (**Fig. 2**). The measurement unit for the total amount is set next to the total amount value (**Fig. 3**). Please note that the selected measurement unit (t/h, kg/h or Nm^3/h) will determine the composition percentage unit (wt % or vol %).

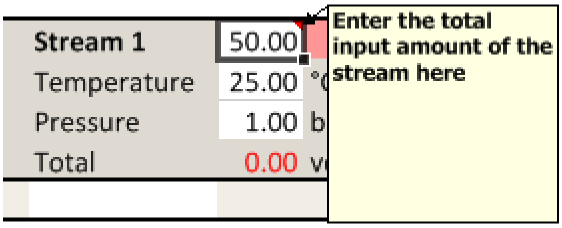


Fig. 2. Total amount of the stream.

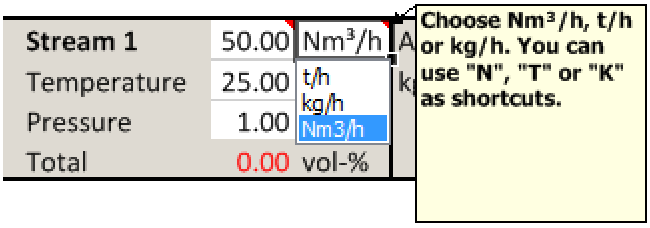


Fig. 3. Measurement unit for the total amount.

The temperature and pressure values can be changed from the cells below the total amount (**Fig. 4**).

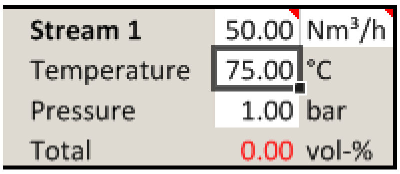


Fig. 4. Temperature and pressure of the stream.

41.2.2. Species and Composition

The species of the stream are entered in the white cells below the stream's header rows (**Fig. 5**).

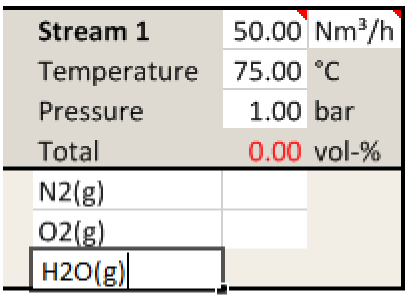


Fig. 5. Enter species in the streams.

Once all the species have been entered, then the composition can be specified (**Fig. 6**). Please pay attention to the composition percentage units.

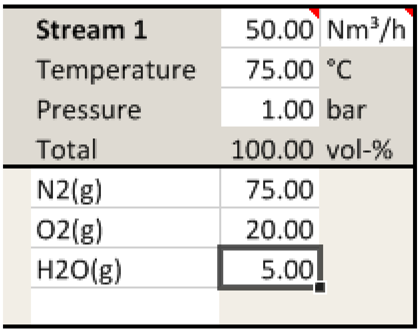


Fig. 6. Composition of a stream.

The above steps need to be repeated for all of the input streams which act as raw material inputs. If an input stream is not a raw material input but a stream from another unit, then the properties of this stream cannot be edited on the Input sheet of the destination unit. The energy feeds (or heat losses) can be entered in the streams using the buttons in the left-hand panel (**Fig. 7**).

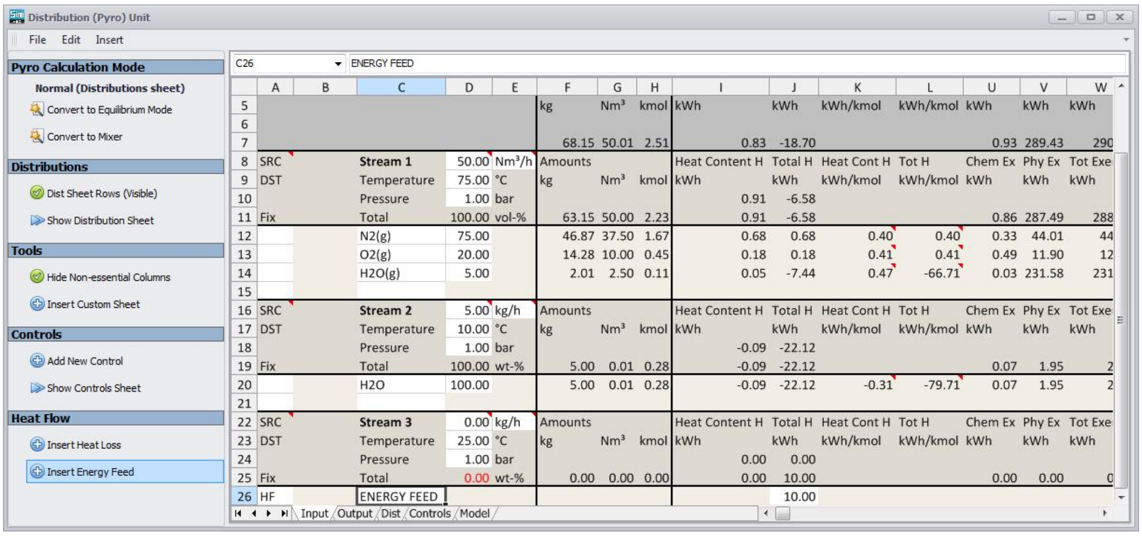


Fig. 7. Inserting an energy feed into a stream.

41.3. Specify Output Streams

On the Output sheet, the same steps need to be carried out as those done for the Input sheet, with the exception of specifying the total amounts and the stream compositions (**Fig. 8**). The amounts and compositions of the output streams are usually specified on the Dist sheet, but there are also wizards which can be used to specify these properties. Specifying the distribution is introduced in section 41.4.

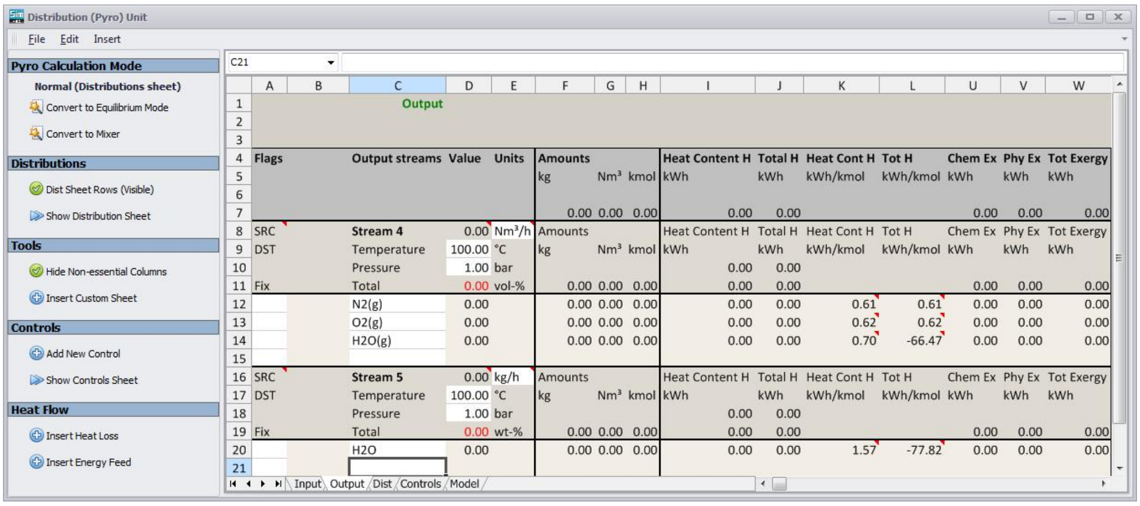


Fig. 8. The user needs to specify: the measurement unit for the amounts, temperature, pressure, and the species for the output streams.

41.4. Specify Distribution

The distribution of the elements from the Input sheet to the Output sheets can be done by using the Dist sheet or by using the Mixer or Equilibrium wizards.

41.4.1. Dist Sheet

You can create the distribution manually by filling the Dist sheet, which is synchronized with the Output sheet. The elements need to be distributed to the streams and the species within those streams. Therefore, the common approach is to first distribute the elements to streams, and then to species. For instance, in this example, the elements H, N and O need to be distributed to two streams. The first stream contains gaseous species (N2(g), O2(g) and H2O(g)) and the second stream contains pure water (H2O) (**Fig. 9**).

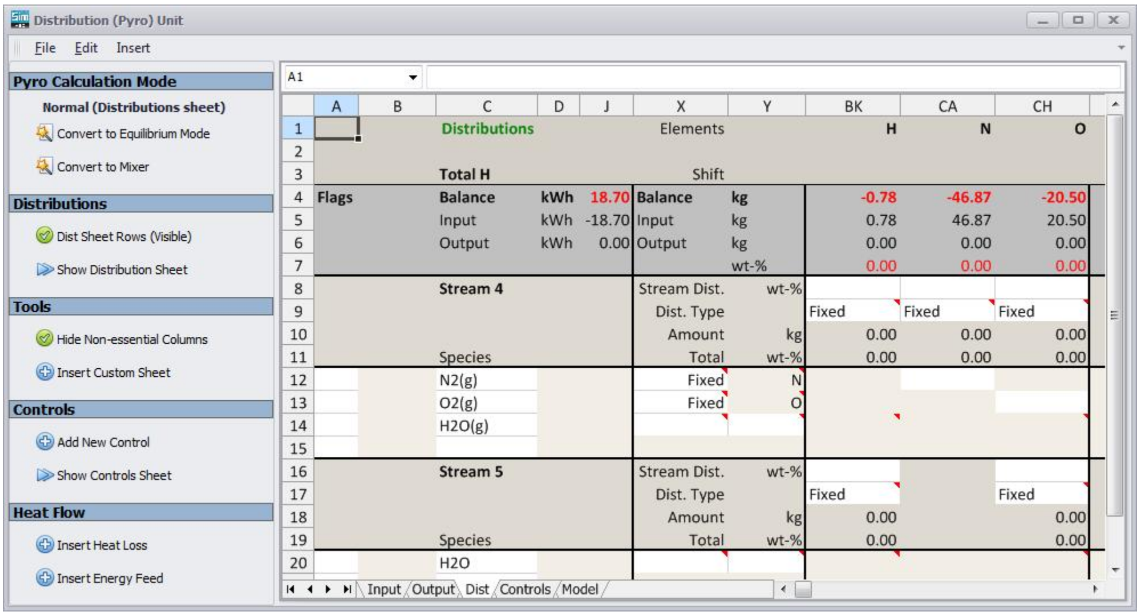


Fig. 9. Dist sheet.

The types of distribution of elements to streams can be Fixed, Rest, and Float:

Fixed - Constant or function value is used.
Rest - All the rest of the element goes into this stream.
Float - Automatically fixed by other elements.

In this example, all the nitrogen is distributed to the first stream and hydrogen and oxygen are distributed to both streams. For instance, it can be initially set that 60% of hydrogen is distributed to the first stream and the rest to the second stream. For oxygen, the distribution type in the second stream will be set as "Float" and "Rest" in the first stream (**Fig. 10**).

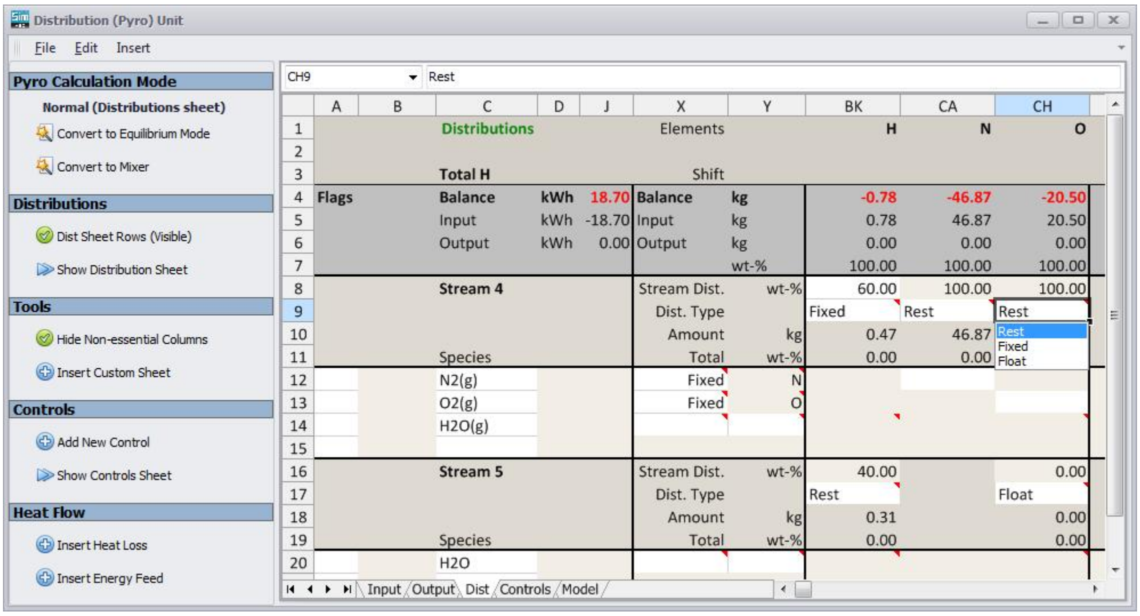


Fig. 10. Distribution of elements to streams.

Next, the elements in the streams will be distributed to the available species. All the species within a stream need to be assigned an element in column Y and a "Fixed" or "Rest" value in column X, which shows how the element amount is distributed to the species.

In this example, H2O can be assigned with all of the hydrogen distributed to the second stream. For the stream with gaseous species, all of the nitrogen will be distributed to the N2(g), all of the hydrogen to the H2O(g), and the remaining oxygen to the O2(g) (**Fig. 11**).

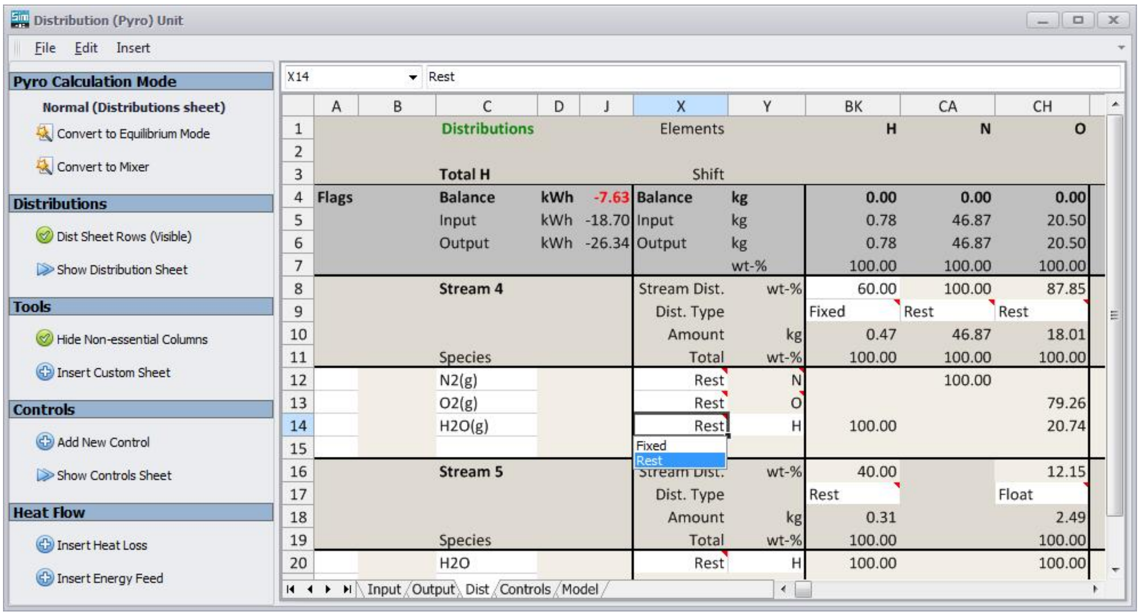


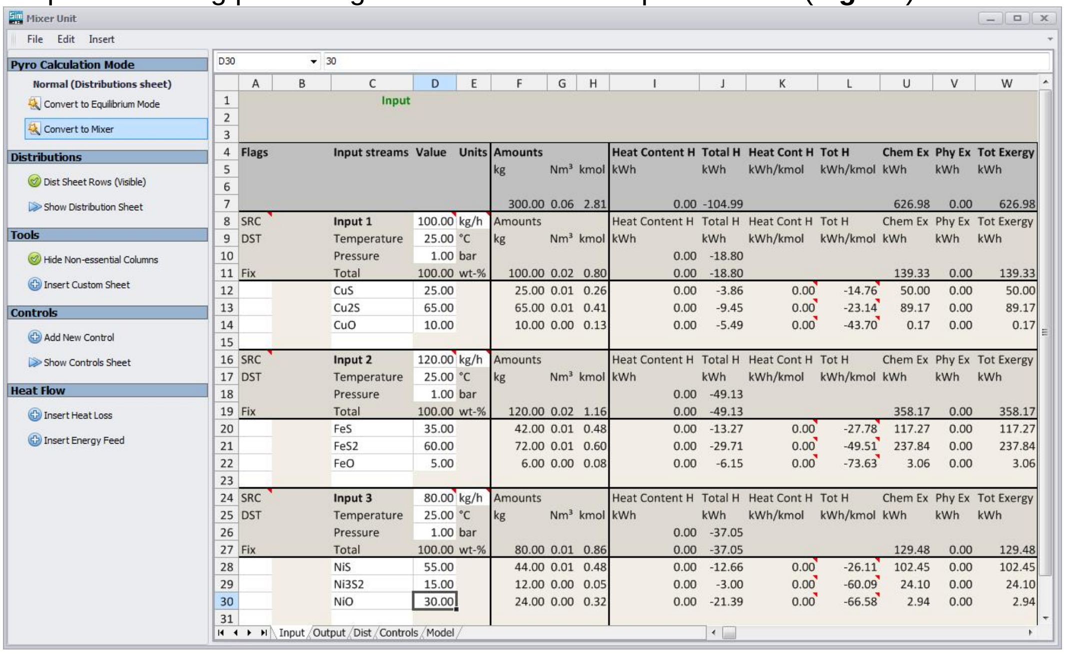
Fig. 11. Elements distributed to species.

NB! When all the elements have been correctly distributed to the species, the element balance, on row 4, should show zero values for all the elements. This ensures that all the atoms are conserved in the distribution unit.

41.4.2. Mixer Wizard

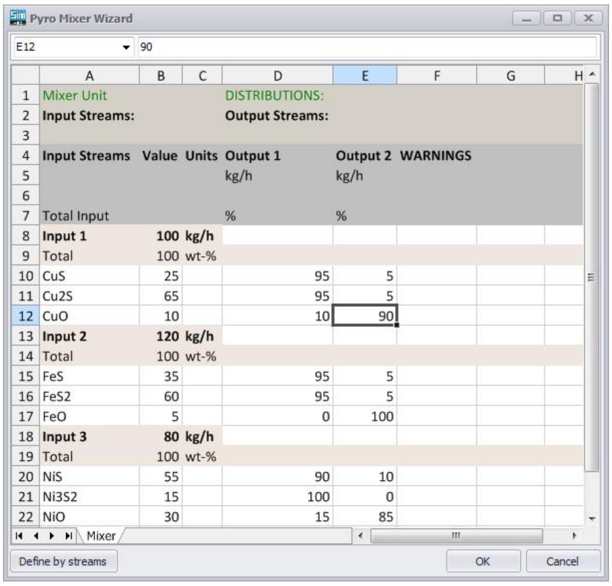
If the unit operation does not include any reactions between the species, then the species can be distributed directly to the output streams with the Mixer wizard. For the Mixer wizard, you do not need to specify the species for the Output sheet, but you need to specify the measurement unit for the amounts. Please also note that the Mixer wizard requires that the same measurement unit is used for all the streams (both input and output).

The Mixer wizard option is found on the left-hand panel (**Fig. 12**). Distribution in the wizard is specified using percentages for each of the output streams (**Fig. 13**).



	A	C	D	E	F	G	H	I	J	K	L	U	V	W
4	Flags	Input streams	Value	Units	Amounts			Heat Content H	Total H	Heat Cont H	Tot H	Chem Ex	Phy Ex	Tot Exergy
5					kg	Nm³	kmol	kWh	kWh	kWh/kmol	kWh/kmol	kWh	kWh	kWh
7					300.00	0.06	2.81	0.00	-104.99			626.98	0.00	626.98
8	SRC	Input 1	100.00	kg/h	Amounts			Heat Content H	Total H	Heat Cont H	Tot H	Chem Ex	Phy Ex	Tot Exergy
9	DST	Temperature	25.00	°C	kg	Nm³	kmol	kWh	kWh	kWh/kmol	kWh/kmol	kWh	kWh	kWh
10		Pressure	1.00	bar				0.00	-18.80					
11	Fix	Total	100.00	wt-%	100.00	0.02	0.80	0.00	-18.80			139.33	0.00	139.33
12		CuS	25.00		25.00	0.01	0.26	0.00	-3.86	0.00	-14.76	50.00	0.00	50.00
13		Cu2S	65.00		65.00	0.01	0.41	0.00	-9.45	0.00	-23.14	89.17	0.00	89.17
14		CuO	10.00		10.00	0.00	0.13	0.00	-5.49	0.00	-43.70	0.17	0.00	0.17
16	SRC	Input 2	120.00	kg/h	Amounts			Heat Content H	Total H	Heat Cont H	Tot H	Chem Ex	Phy Ex	Tot Exergy
17	DST	Temperature	25.00	°C	kg	Nm³	kmol	kWh	kWh	kWh/kmol	kWh/kmol	kWh	kWh	kWh
18		Pressure	1.00	bar				0.00	-49.13					
19	Fix	Total	100.00	wt-%	120.00	0.02	1.16	0.00	-49.13			358.17	0.00	358.17
20		FeS	35.00		42.00	0.01	0.48	0.00	-13.27	0.00	-27.78	117.27	0.00	117.27
21		FeS2	60.00		72.00	0.01	0.60	0.00	-29.71	0.00	-49.51	237.84	0.00	237.84
22		FeO	5.00		6.00	0.00	0.08	0.00	-6.15	0.00	-73.63	3.06	0.00	3.06
24	SRC	Input 3	80.00	kg/h	Amounts			Heat Content H	Total H	Heat Cont H	Tot H	Chem Ex	Phy Ex	Tot Exergy
25	DST	Temperature	25.00	°C	kg	Nm³	kmol	kWh	kWh	kWh/kmol	kWh/kmol	kWh	kWh	kWh
26		Pressure	1.00	bar				0.00	-37.05					
27	Fix	Total	100.00	wt-%	80.00	0.01	0.86	0.00	-37.05			129.48	0.00	129.48
28		NiS	55.00		44.00	0.01	0.48	0.00	-12.66	0.00	-26.11	102.45	0.00	102.45
29		Ni3S2	15.00		12.00	0.00	0.05	0.00	-3.00	0.00	-60.09	24.10	0.00	24.10
30		NiO	30.00		24.00	0.00	0.32	0.00	-21.39	0.00	-66.58	2.94	0.00	2.94

Fig. 12. Using the Mixer wizard.



	A	B	C	D	E	F
1	Mixer Unit			DISTRIBUTIONS:		
2	Input Streams:			Output Streams:		
4	Input Streams	Value	Units	Output 1	Output 2	WARNINGS
5				kg/h	kg/h	
7	Total Input			%	%	
8	**Input 1**	**100**	**kg/h**			
9	Total	100	wt-%			
10	CuS	25		95	5	
11	Cu2S	65		95	5	
12	CuO	10		10	90	
13	**Input 2**	**120**	**kg/h**			
14	Total	100	wt-%			
15	FeS	35		95	5	
16	FeS2	60		95	5	
17	FeO	5		0	100	
18	**Input 3**	**80**	**kg/h**			
19	Total	100	wt-%			
20	NiS	55		90	10	
21	Ni3S2	15		100	0	
22	NiO	30		15	85	

Fig. 13. Distributing species with the Mixer wizard.

41.4.3. Equilibrium Wizard

The composition of output streams can also be calculated with the Equilibrium wizard. This allows you to distribute the elements from the input sheet to species in the Output streams, based on their chemical stability at the specified output temperature.

The Equilibrium wizard option is found on the left-hand panel (**Fig. 14**) and the equilibrium results are presented on the Gibbs sheet, which is linked to the Output sheet. You need to specify the Input sheet as well as the Output sheet for the wizard. The streams on the Output sheet are assumed to be separate phases in the equilibrium calculations (**Fig. 15**). Phases can be set either as a mixture or as pure phases.

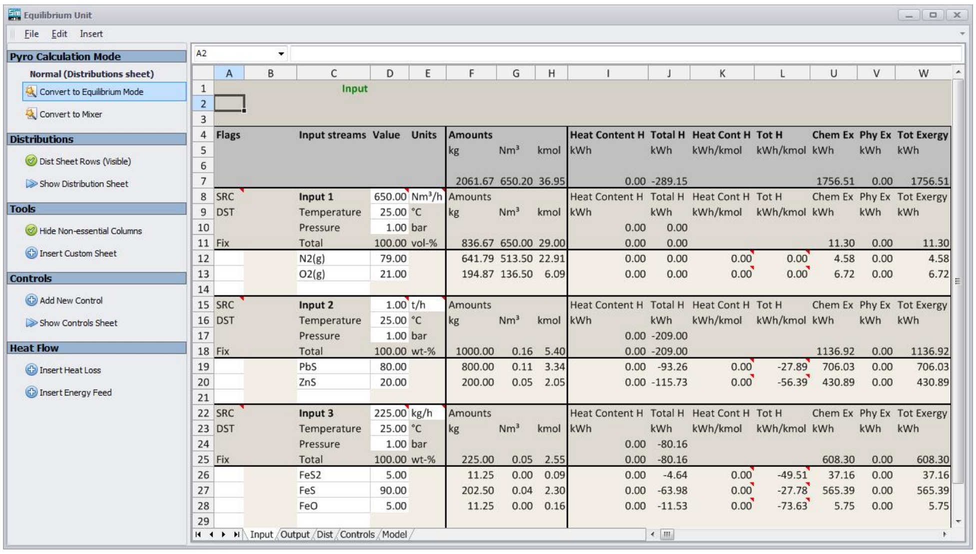


Fig. 14. Using the Equilibrium wizard.

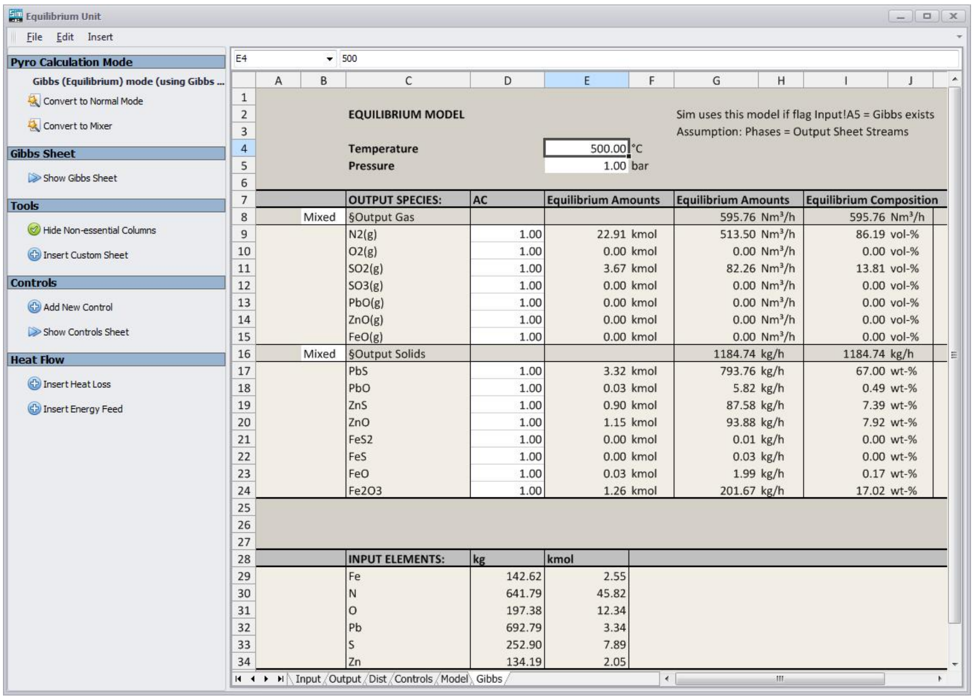


Fig. 15. Distributing elements with the Equilibrium wizard.

41.5. Set Controls

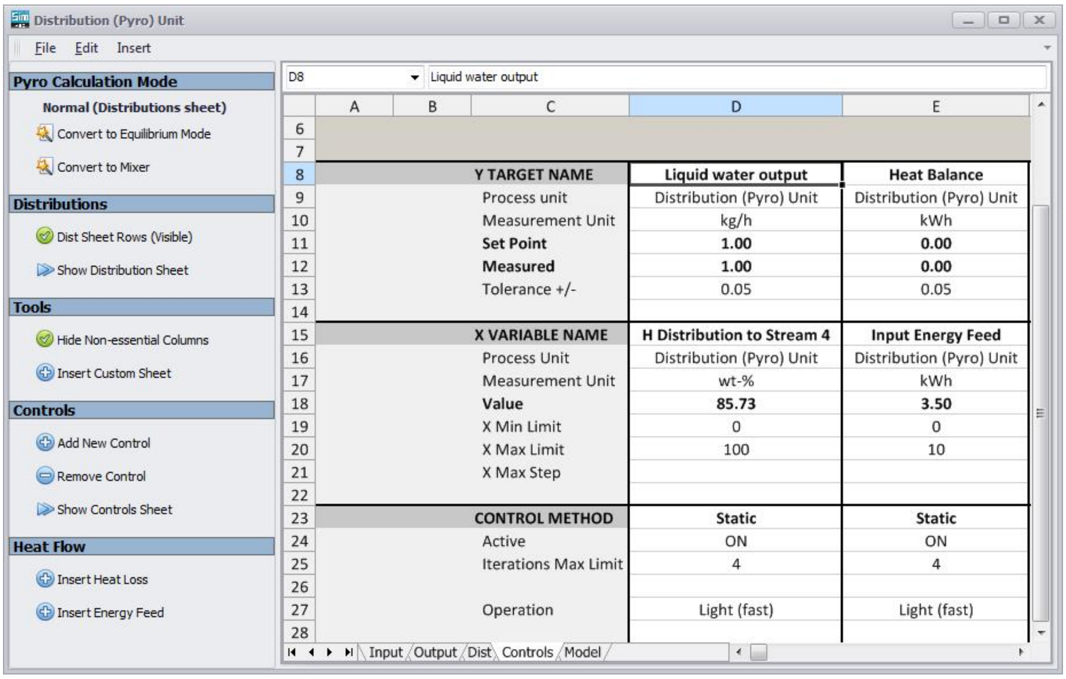


Fig. 16. Controls sheet with two controls.

The HSC Sim Controls sheet makes it possible to create controls that regulate the target parameter cell value using another variable cell value, **Fig. 16**. In principle, Sim Control works exactly like a real process control. For example, in a real process unit you can give a set point to the process unit temperature and regulate the temperature by changing the fuel oil feed.

To create a control on the Controls sheet, you have to set at minimum the Set Point, the Target cell reference, Variable cell reference, the limits for the variable, and the tolerance. You can type this information on the Controls sheet using the following procedure:

1. Type the name and the measurement unit into Controls sheet cells D9 to D10 (optional).
2. Type the Target set value (Set Point) into cell D11.
3. Locate the Target cell in your active unit and right-click "Copy cell reference".
4. Go to Controls sheet cell D12 and right-click "Paste cell reference".
5. Give the tolerance of the calculation in cell D13. When the difference of Set Point and Measured value is smaller than the Tolerance, the control is in balance and will not be calculated further.
6. Type the name and the unit of measure in cells D16 and D17 (optional).
7. Locate the Variable cell in your active unit and select "Copy cell reference".
8. Go to Controls sheet cell D18 and right-click "Paste cell reference".
9. Type **Limit Min** and **Max** in cells D19 and D20, a narrow numerical range speeds up the calculations.

The default **Tolerance** is +/-. A small tolerance increases the calculation time and a large tolerance increases errors. Some 2% of the target value may be a good compromise. The control will not be taken into account if the value is within the tolerance.

Sim Controls have exactly the same **limitations** as real process controls, for example:

- If the target cell does not depend on the variable cell value, the iterations will fail.
- If an external variable cell is used, there may be a long delay before the effect on the target value becomes visible. In these cases a lot of iteration rounds might be needed to reach the Set Point. This increases the calculation time.

Table 1. Information on the Controls sheet.

Row	**Name**	**Description**
8	Y Target Name	Name of Y (optional)
9	Process Unit	Unit name (optional)
10	Measurement Unit	Name of the unit of measure (optional)
11	**Set Point**	**Set point of Y (obligatory)**
12	**Measured**	**Y cell reference (obligatory)**
13	**Tolerance +/-**	**Y tolerance (obligatory)**
15	X Variable Name	Name of X (optional)
16	Process Unit	Unit name (optional)
17	Measurement Unit	Name of the unit of measure (optional)
18	**Value**	**X cell reference (obligatory)**
19	**X Min Limit**	**Min limit of the X range (obligatory)**
20	**X Max Limit**	**Max limit of the X range (obligatory)**
21	X Max Step	Maximum X Step (optional, default = empty)
23	Control Method	Iteration method (optional, default = Auto[1])
24	Active	Set control ON/OFF (optional, default = empty = ON)
25	Iterations max limit	Max number of iterations (optional, default = 10)
26	Iterations min limit	Min number of iterations (optional, default = empty)
27	Operation	Control calculation operation (optional, default = Light[2])

[1]**Auto** (Solves the control with information on rows 24 - 27), **Auto Smart** (Same as Auto except changes X Max Step and Iterations max limit when needed), **PID** (not in use, will be added to the HSC8 version).

[2]**Light** (Solves the control with modified tangent method, fast), **Robust** (Solves the control with modified Newton method, slow), **Simple direct** (Increases X value when Measured value is too small. The step used can be specified in X max step.), **Simple reverse** (Decreases X value when Measured value is too small. The step used can be specified in X max step.).

41.5.1. Internal and External Controls

1. Internal control in which the target and variable cells exist in the same process unit (FAST).

2. External control in which the target and variable cells exist in different process units (SLOW).

Calculation of an internal control is fast because only one unit is calculated. Usually you can create a large number of **internal controls** in a process without a dramatic drop in calculation speed, because they do not increase the number of calculation rounds of the process.

Calculation of an external control might take more time because material must be recirculated within the whole process several times to reach a stable target value. Usually only a few **external controls** can be used in one process without a considerable decrease in the calculation speed, because external controls might multiply the calculation rounds of the process.

41.5.2. Advice When Using Controls

- It is recommended to moderate large changes of the variable with the use of **X Max Step**, when using external controls with slow responses.
- The **RecoveryX** add-in function cannot be used in the Target cell, because it is recalculated only after all the calculation rounds have been completed.
- The large number of thermochemical add-in functions (**StreamH**, **StreamS**, etc.) may reduce the calculation speed if the argument value changes in each control iteration round, because the data search from the H, S, and Cp database takes time. Use these add-in functions only when necessary.

42. Sim Distribution Example

Magnetite Oxidation Example

Pelletized magnetite (Fe_3O_4) ore can be oxidized to hematite (Fe_2O_3) in a shaft furnace. The typical magnetite content of the ore is approx. 95%. Oxidation is usually done by feeding air into the shaft furnace. Some excess oxygen is needed to complete the reaction; the free oxygen in process gas is usually approx. 5%. About 1% of the iron does not react. Coal is used as a fuel to keep the product temperature at 700 °C.

This kind of unit process can be controlled by air and coal feeds. The ore feed can be fixed to approx. 200 t/h. Now, please create a process model of the shaft furnace with oxygen and coal controls.

Walkthrough steps:

1. Draw the flowsheet
2. Draw the streams on the flowsheet
3. Rename the units and streams
4. Save the process
5. Specify the raw material streams
6. Specify the output streams
7. Create a model
    a. Distribution to output streams
    b. Distribution to species within streams
8. Create the controls
9. Run the process model

42.1. Step 1. Draw the flowsheet

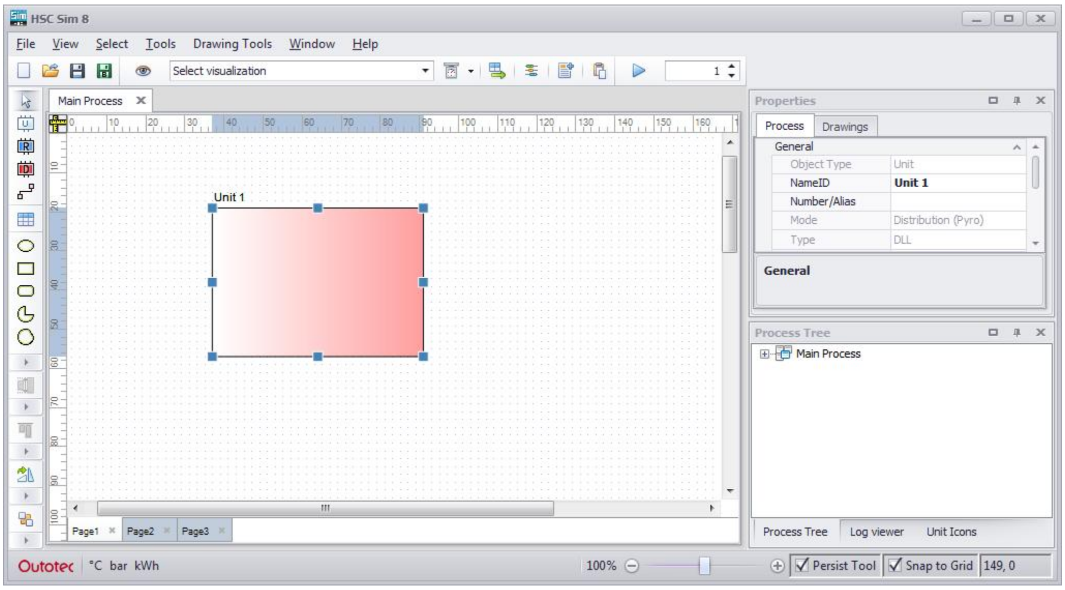


Fig. 1. Draw unit (distribution) on the flowsheet.

First, draw the flowsheet for the process. Usually it is easiest to start with the units of the process (**Fig. 1**). You can draw a generic unit and select its model from the Unit Model Editor, or simply draw a distribution unit by using the red unit icon.

42.2. Step 2. Draw the Streams on the Flowsheet

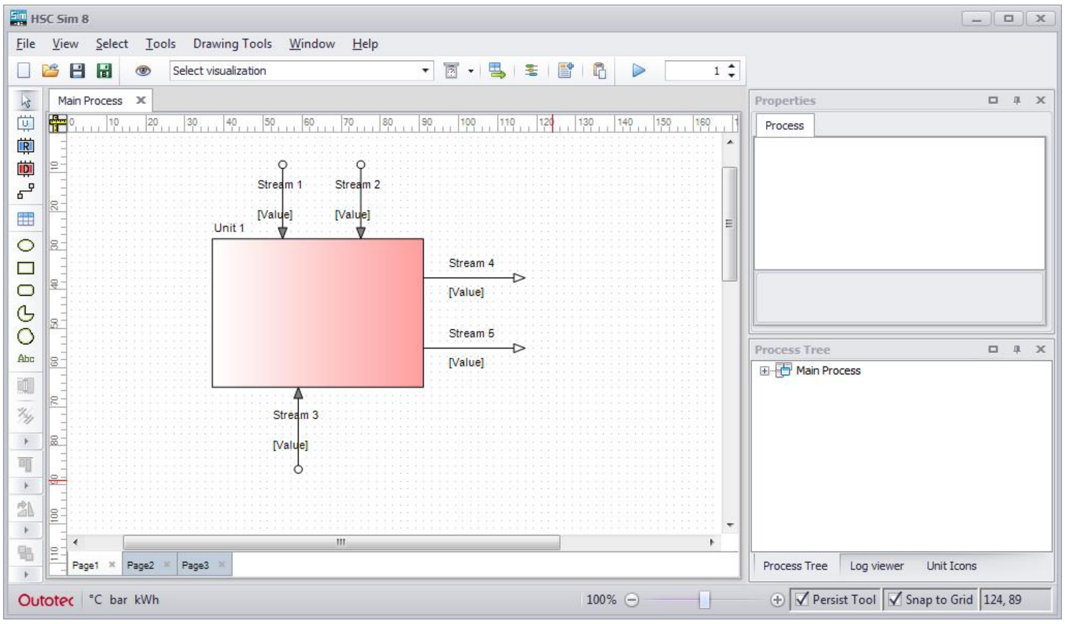


Fig. 2. Draw streams on the flowsheet.

The second step is to draw streams (**Fig. 2**), which must be done using the Stream tool on the left toolbar. The shapes and colors at the end points of the streams indicate their connections. You can also check the Source and Destination units for each stream from the Process tab. If a stream is not connected from either end, then this value is shown as a question mark (?) for the missing Source or Destination value.

Process raw material streams do not have specified Sources, whereas the Destination units are missing for the process output streams. Intermediate streams should have both Source and Destination values specified.

42.3. Step 3. Rename the Units and Streams

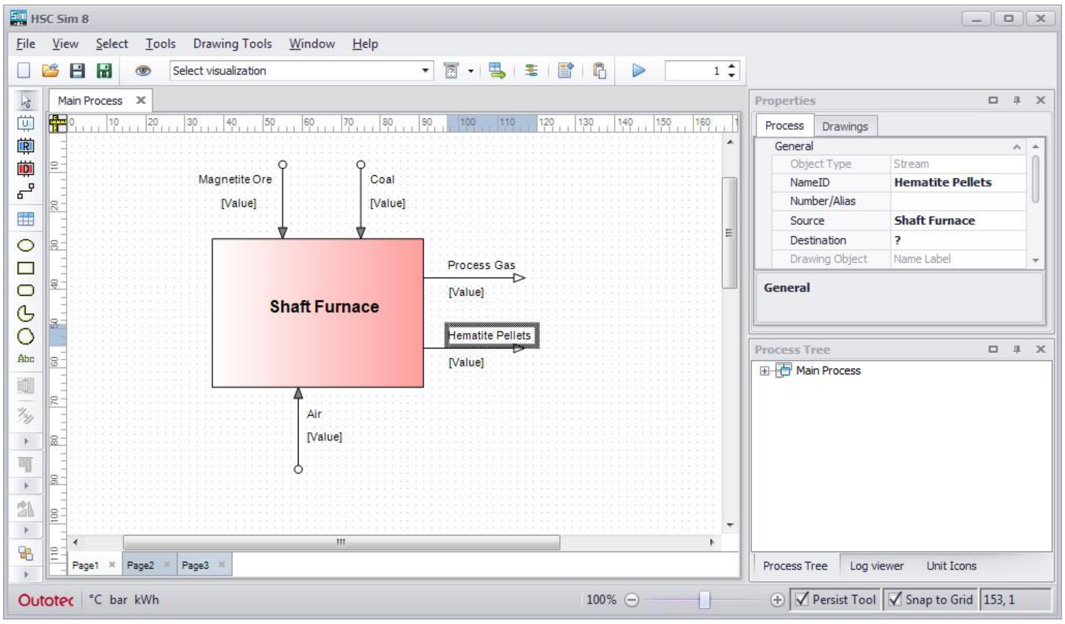


Fig. 3. Renaming units and streams makes flowsheet easier to read.

You can relocate the unit and stream name labels by dragging them with the mouse. Select the unit or stream and rename it using the NameID property. This property is used to identify unit and stream objects. Please use short and illustrative names.

The Drawings tab lets you change the label text formatting. Formatting options can be applied to the labels one by one, or you can select multiple labels and change the formatting for all of them. The Select menu at the top bar offers options to select all certain types of labels from the flowsheet.

42.4. Step 4. Save the Process

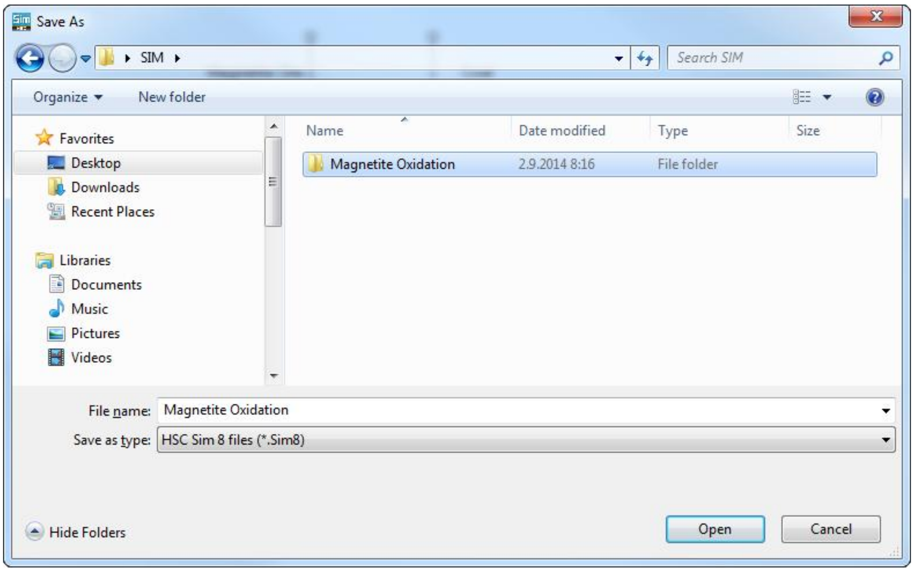


Fig. 4. A process has to have a folder of its own.

It is better to save the process too often rather than too seldom, because a saved process allows you to recover the earlier design stage in case of user or computer errors.

It is necessary to create a separate file folder for each process using the Create New Folder tool, see **Fig. 4**. The process name is also the most logical name for the file folder. In this case the folder name is Magnetite Oxidation and the process name is Magnetite Oxidation. A process can consist of several files and all of these files will be saved into this same folder.

42.5. Step 5. Specify the Raw Material Streams

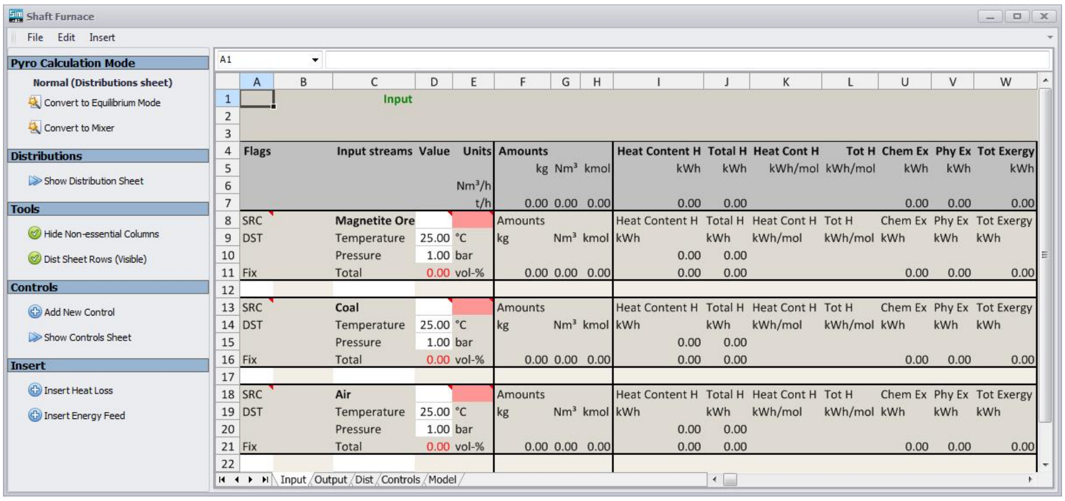


Fig. 5. Raw materials on the Input sheet.

You can open Unit Editor by double-clicking the unit icon on the flowsheet. The raw material streams can be found on the Input sheet. At the beginning these streams are empty. Species can be typed into streams manually.

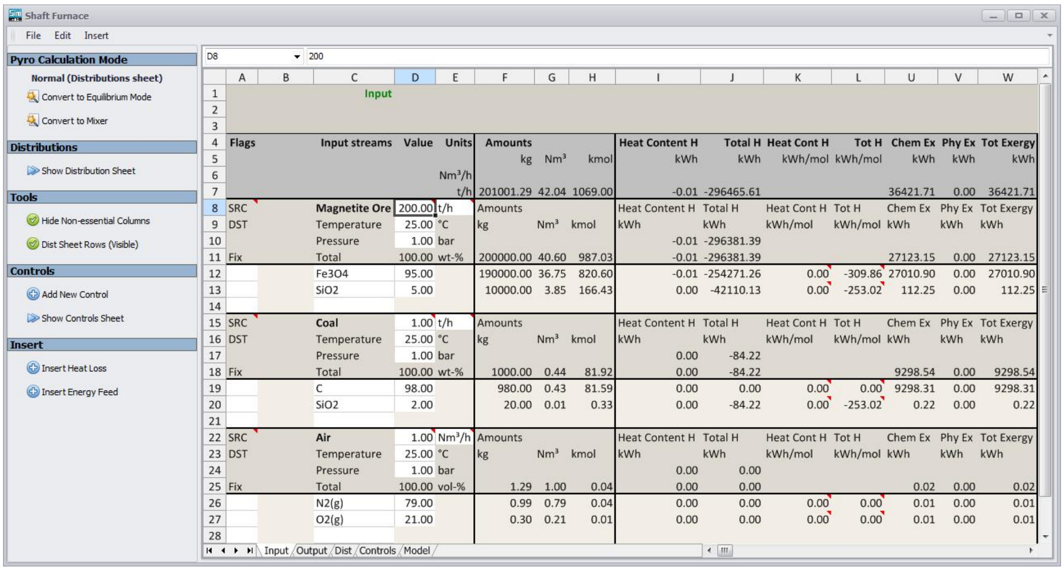


Fig. 6. Specify stream species, compositions, raw material amounts and measure units.

You need to specify the raw material stream species as well as their compositions and temperatures. It is also important to specify the measure units for the streams. Valid selections are:

- t/h
- kg/h
- Nm3/h (only for gases)

Please note that the stream composition is given in wt-%, if mass units are used, and in vol-%, if normal cubic meters are used. If the feed amount is not yet available then it is good to specify an initial value such as 1 t/h, especially if this raw material will be used within some control.

42.6. Step 6. Specify the Output Streams

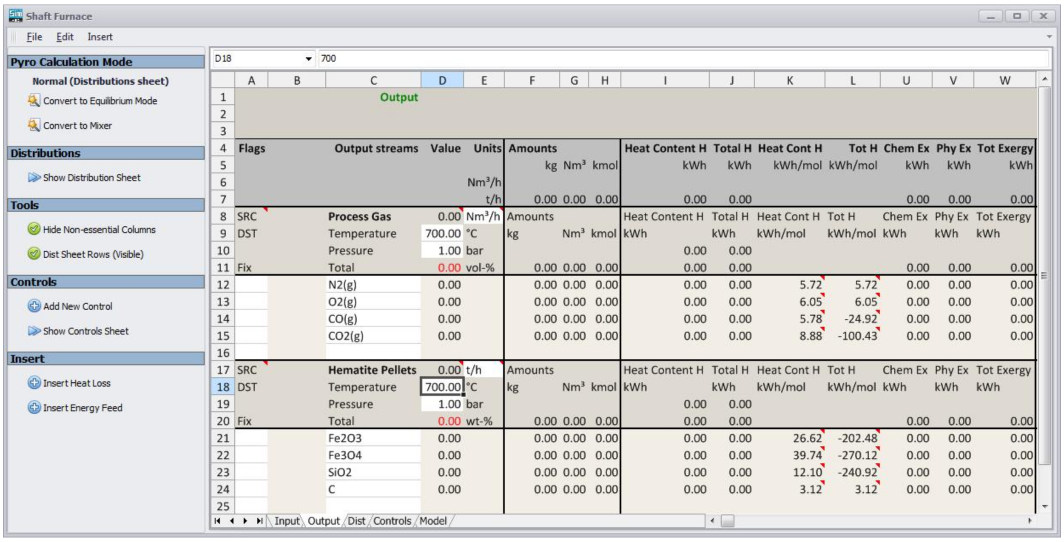


Fig. 7. Output streams are specified on the Output sheet.

You need to specify the species, temperatures, and the measure units of the output streams. Please note that the output stream amounts and species distributions cannot be edited manually, as they will be calculated later.

The Output and Dist sheet streams have been synchronized with each other. This means that when you type species on the Output sheet they will also appear on the Dist sheet.

42.7. Step 7. Create A Model

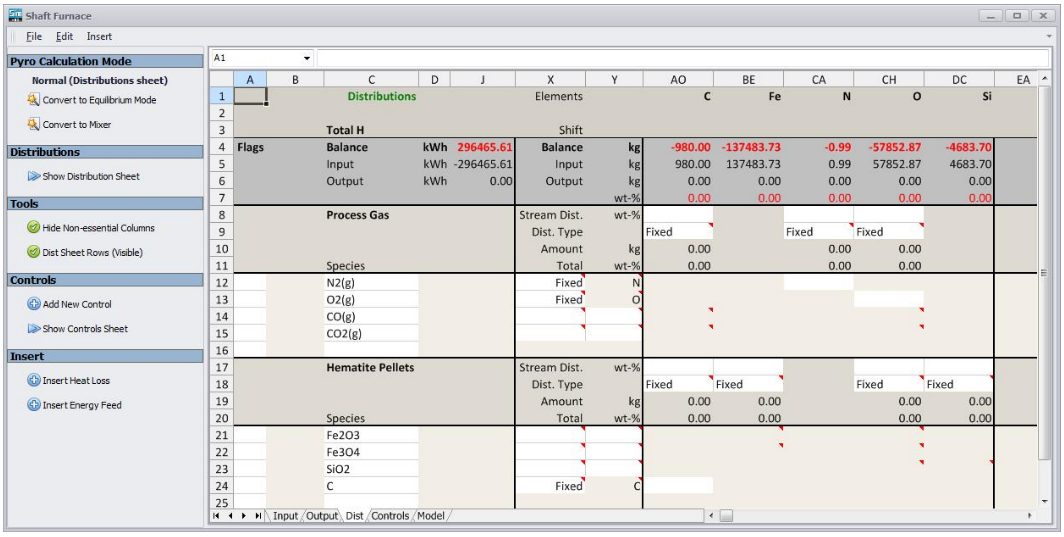


Fig. 8. Element distributions need to be specified on the Dist sheet.

The Sim Distribution mode automatically calculates the total input amounts for the input streams and converts these into elements. The user must specify on the Dist sheet how these elements will be distributed:

a) into output streams
b) into species within one stream

The Popup list tool can be used in the specification procedure. This tool is automatically opened when you click a cell where the operation is possible. The options are:

- **Fixed**
  The distribution is fixed with a constant %-value or an Excel-type formula.
  Only a constant value cell may be used as a variable on the Controls sheet!
- **Rest**
  When all the specifications have been made for a certain element, then the remaining fraction of the element must go to one species and one phase.
- **Float**
  This option means that the current cell has been automatically specified by the other elements like metals. It is usually wise to specify oxygen, sulfur, etc. as floating elements.

42.7.1. Step 7.a - Distribution to Output Streams

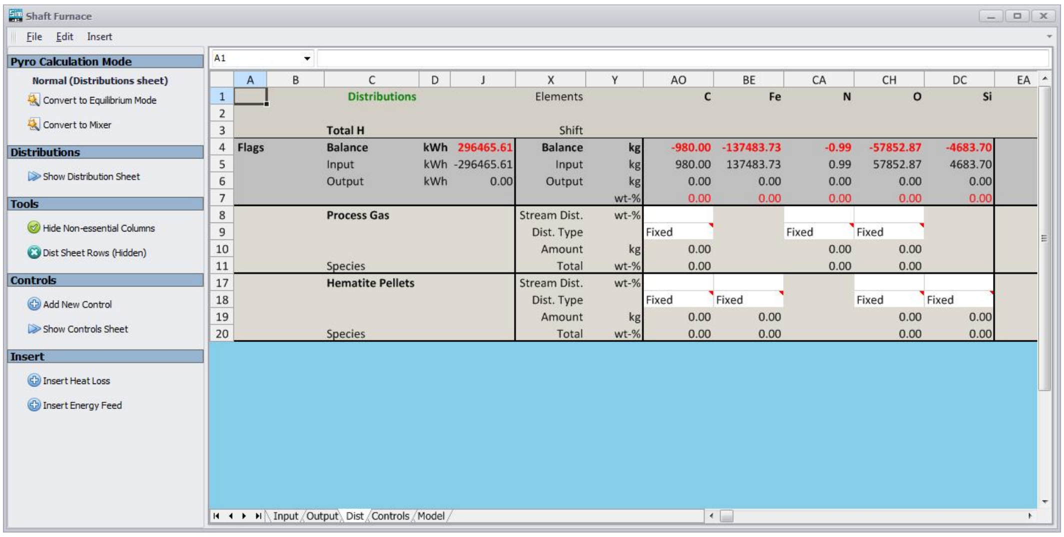


Fig. 9. Distribution to output streams.

When distributing the elements to output streams, it might be helpful to hide the species rows with the "Dist Sheet Rows" button in the left-hand panel (**Fig. 9**).

An easy way to start is to fix the elements which are present only in one stream. In this example, this applies to nitrogen (N), iron (Fe), and silicon (Si). Nitrogen is present only in the "Process Gas" stream, whereas iron and silicon are only found in the "Hematite Pellets" stream. To distribute these elements, set their status to Fixed in the correct streams and give their wt-% value as 100 (**Fig. 10**). Note that you can also use the Rest status for the elements that are found only in one stream.

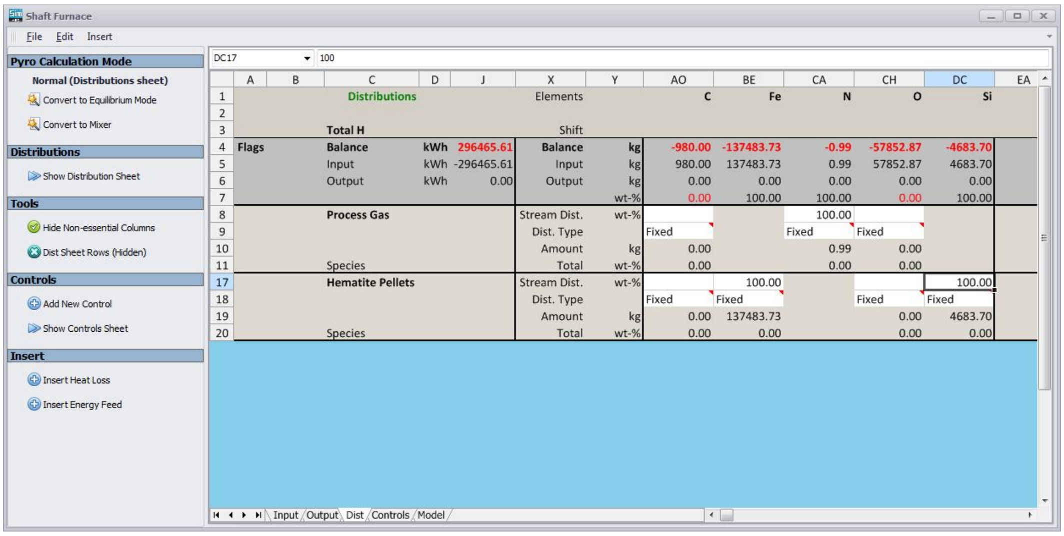


Fig. 10. Fixing elements (N, Fe, and Si) in the output streams.

For elements that are present in several streams, distribution can be done e.g. by fixing a value for one stream and letting the remaining amount go to the other. For example, you can define that 0.1 wt-% of carbon (C) goes into the "Hematite Pellets" stream and the rest will be distributed to the "Process Gas" stream. To do this, set the status of carbon to Fixed in the "Hematite Pellets" stream and give the wt-% value as 0.1, then set the status of carbon in the "Process Gas" stream as Rest (**Fig. 11**).

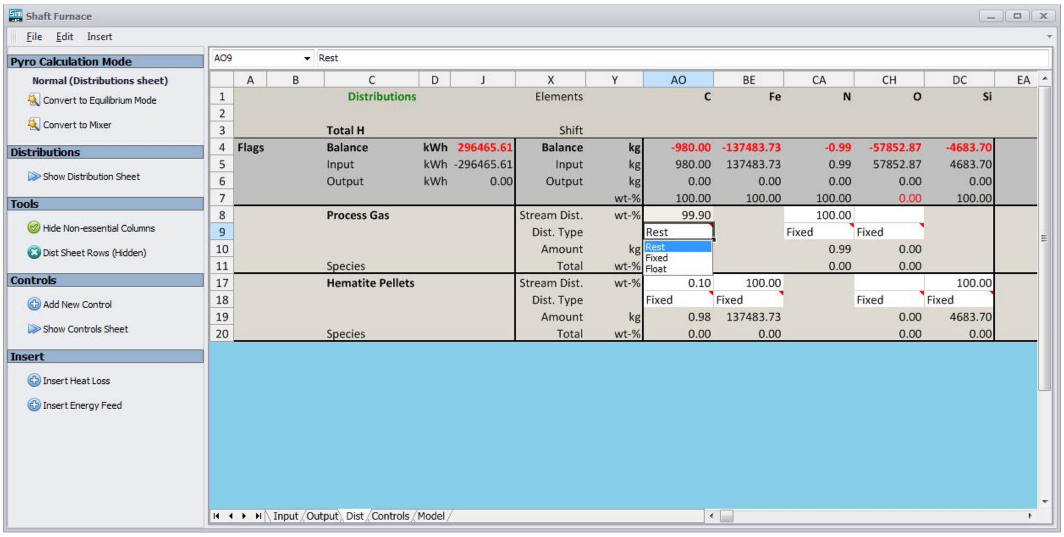


Fig. 11. Fixed fraction of carbon in the pellets stream and rest in the gas stream.

Finally, oxygen needs to be distributed to the output streams. In the "Hematite Pellets" stream, oxygen is present in iron oxides and silica. By letting the iron and silicon content of the pellet stream determine the amount of oxygen, the status can be set as Float. The rest of the oxygen will be distributed to the "Process Gas" stream by setting the status as Rest (**Fig. 12**).

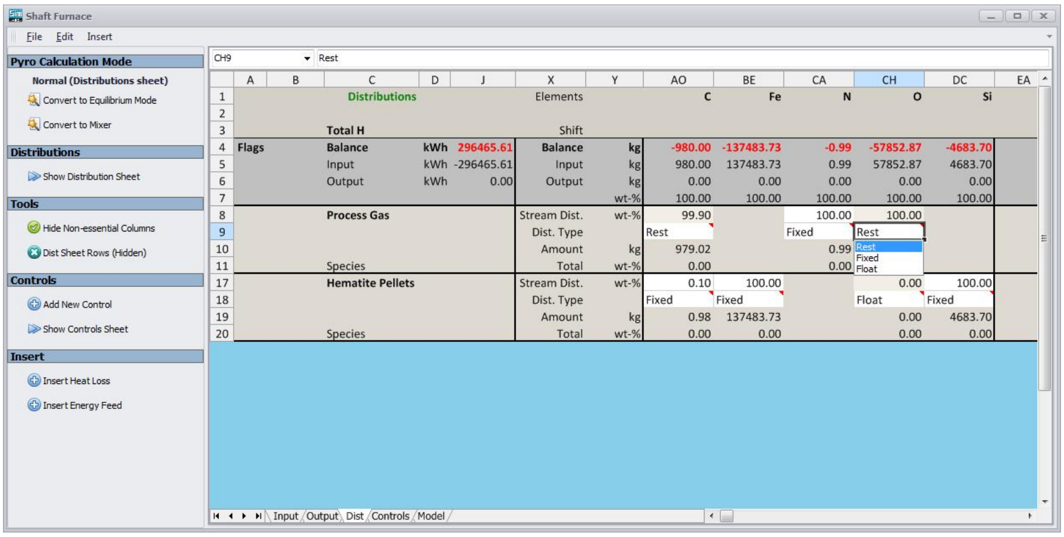


Fig. 12. Distribution of oxygen to output streams.

Please note that after the elemental distribution to the output streams is finished, the wt-% values in row 7 should all be 100.

42.7.2. Step 7.b - Distribution to Species within Streams

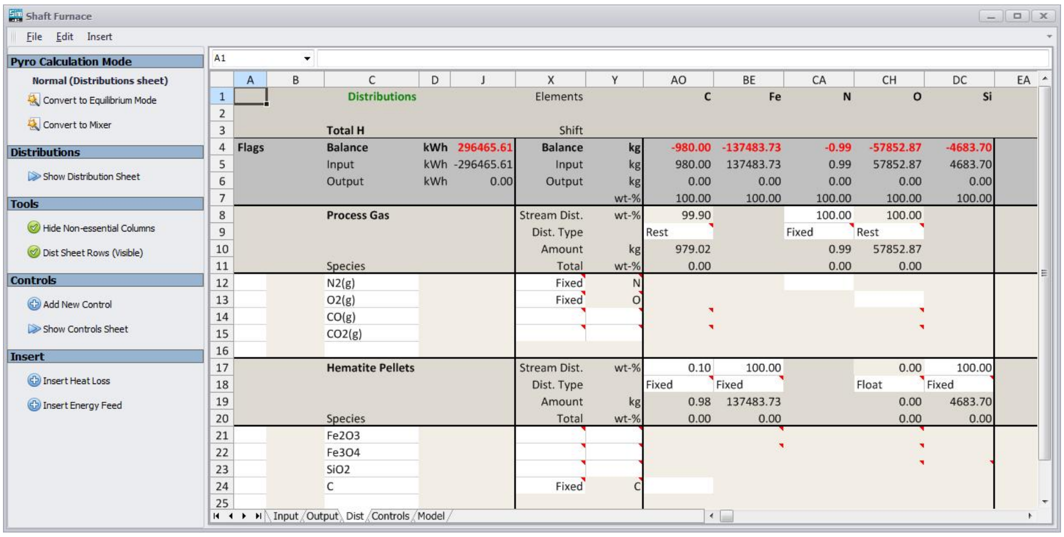


Fig. 13. Distribution of elements to species.

All the species in the streams need to be assigned with an element in column Y and a status in column X. These parameters together are used to distribute the elements to species. Species that contain only a single element have their element assigned automatically.

In the "Hematite Pellets" stream, it is easiest to start with carbon (C) and silica (SiO_2). For carbon atoms, there is only one species (C), so this species can be assigned to contain 100% of the stream's carbon content. Similarly, you can fix the silica amount by assigning the species to the element Si, and setting the species to contain 100% of the stream's silicon content (**Fig. 14**).

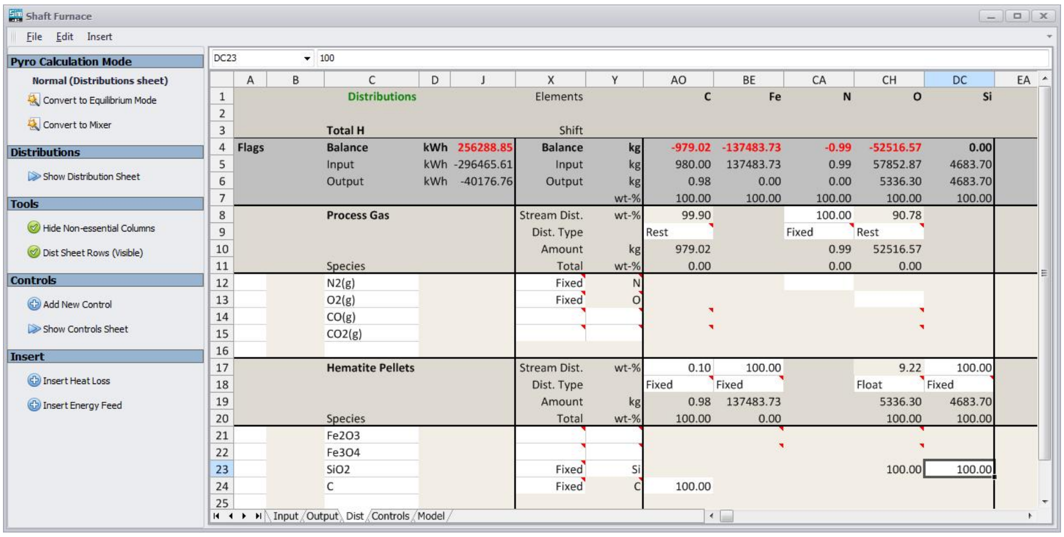


Fig. 14. Carbon and silicon distribution in the pellets stream.

Iron is distributed between magnetite (Fe3O4) and hematite (Fe2O3). In this example, it is assumed that almost all of the magnetite is oxidized. This can be simulated by fixing 1% of stream's iron content to Fe3O4 and distributing the rest to Fe2O3 (**Fig. 15**).

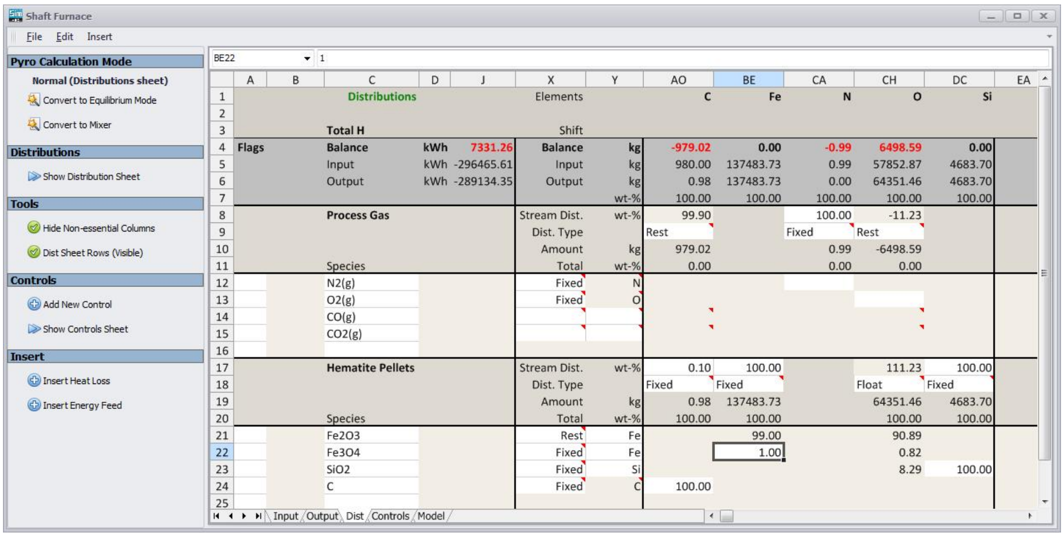


Fig. 15. Iron distribution to the pellets stream.

Next, the elements can be distributed to the "Process Gas" stream. Again, an easy way to start is to distribute the nitrogen (N) atoms to the only species (N2(g)) which contains nitrogen (**Fig. 16**).

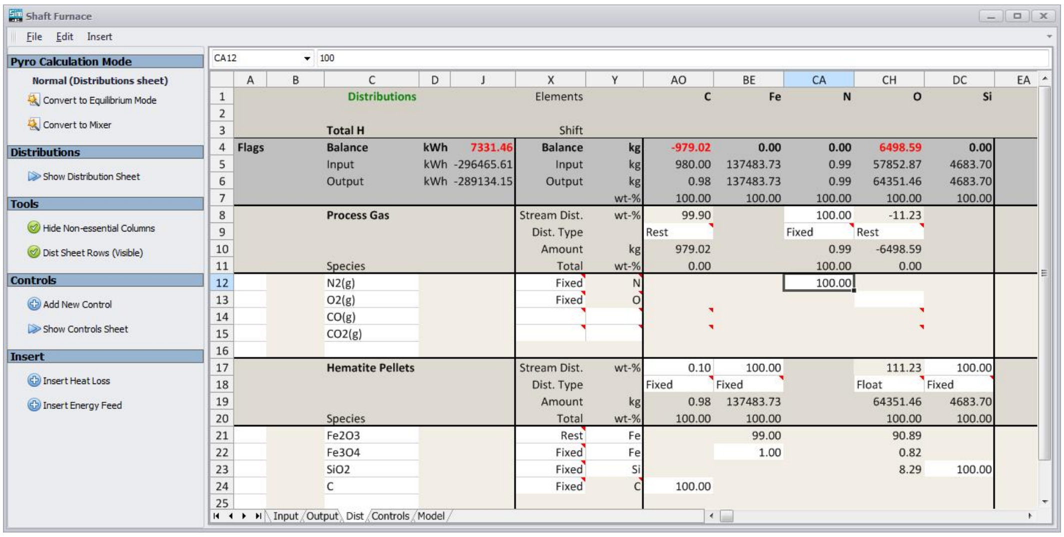


Fig. 16. Nitrogen distribution in the gas stream.

For the carbon-containing species (CO(g) and CO2(g)), it can be assumed that enough oxygen is provided for all of the carbon in the gas stream to be oxidized into carbon dioxide. Thus, carbon (C) can be assigned to both species and the CO(g) will be fixed at 0.00, and for CO2(g) the status can be set as Rest (**Fig. 17**).

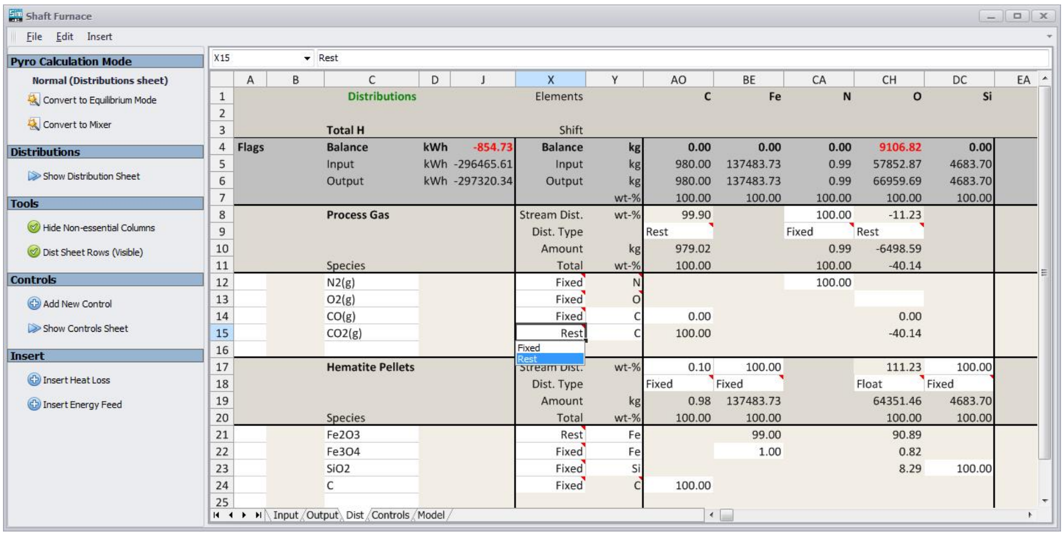


Fig. 17. Carbon distribution in the gas stream.

The final thing to do is to distribute all excess oxygen atoms (O) to oxygen gas (O2(g)). This can be done by setting the status to Rest (**Fig. 18**).

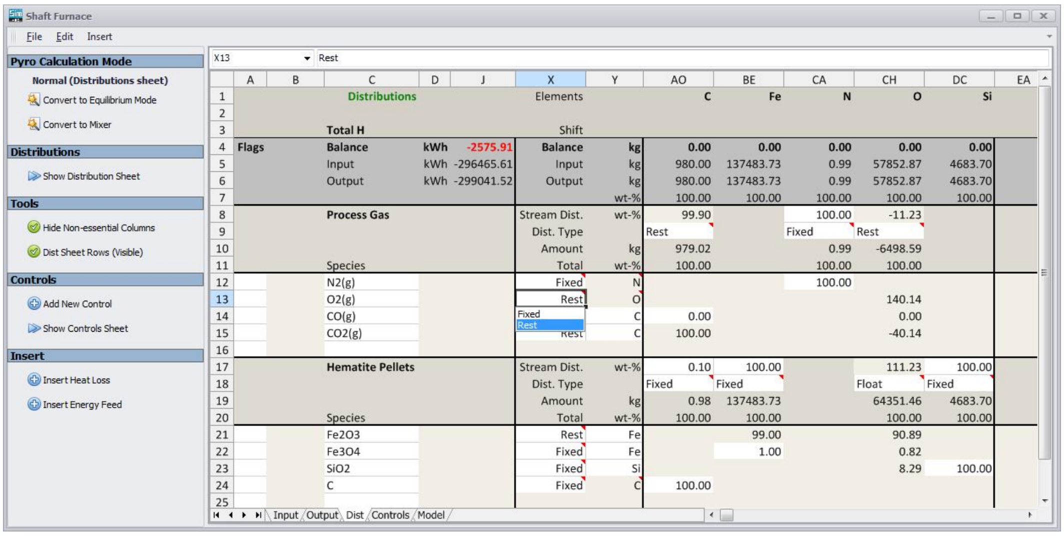


Fig. 18. Oxygen distribution in the gas stream.

Now the distribution of elements in the output streams is ready. It is important to notice that for a correctly filled Dist sheet, the Balance value for all of the elements is equal to zero (**Fig. 19**). This indicates that all the atoms are conserved, and thus the elemental balance is maintained.

	A	B	C	D	J	X	Y	AO	BE	CA	CH	DC
1			Distributions			Elements		C	Fe	N	O	Si
2												
3			Total H			Shift						
4	Flags		Balance	kWh	-2575.91	Balance	kg	0.00	0.00	0.00	0.00	0.00
5			Input	kWh	-296465.61	Input	kg	980.00	137483.73	0.99	57852.87	4683.70
6			Output	kWh	-299041.52	Output	kg	980.00	137483.73	0.99	57852.87	4683.70
7							wt-%	100.00	100.00	100.00	100.00	100.00

Fig. 19. Zero values indicate that all the atoms are conserved.

42.8. Step 8. Create the Controls

Controls are often used to regulate distribution values, output stream compositions and heat balances. For each control we have to specify:

1) A target cell and a Set Point value for this cell
2) A variable cell used to regulate the target cell

The variable cell must have some effect on the target cell parameter. If this is not true, then the control will not work. The situation is exactly the same when you control real processes and plants.

In this example two controls are used: one to regulate the O2 content in the "Process Gas" stream, and another to ensure that the heat balance is maintained.

First, add two controls to the sheet by clicking the **Add New Control** button in the left-hand panel, and type the name of the first control (**Fig. 20**).

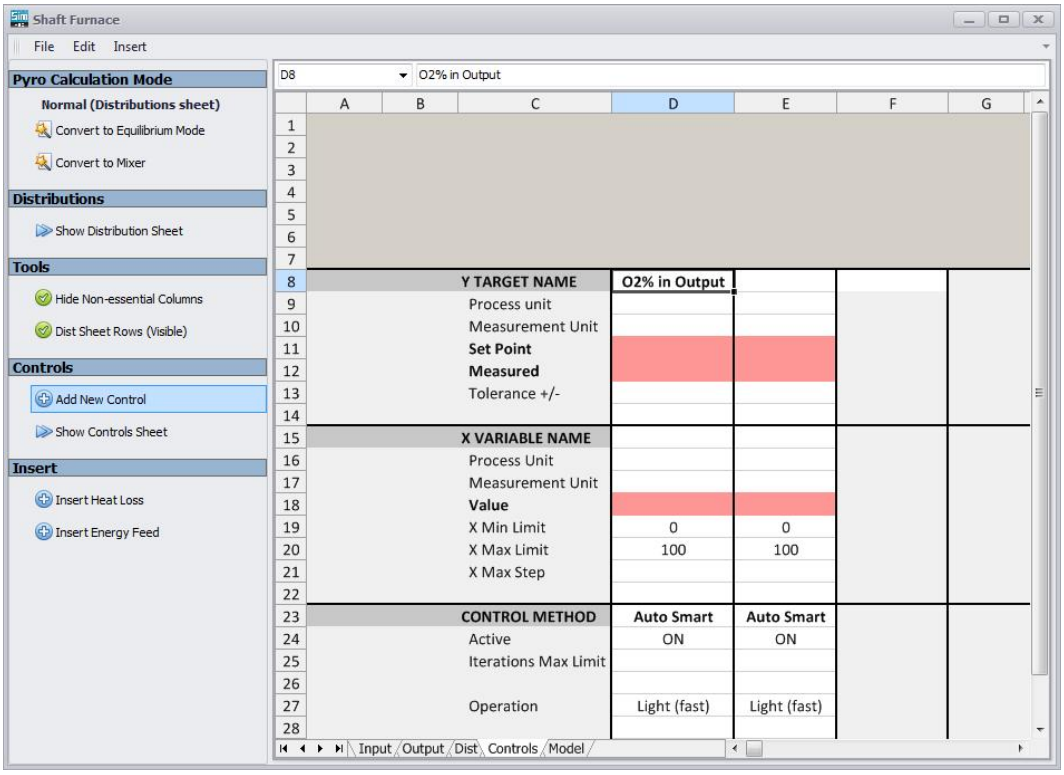


Fig. 20. Controls can be added to the sheet with the Add New Control button.

Next, set the cell reference for the target parameter. For this control, the correct cell can be found on the Output sheet, cell D13 (Output!D13). To set this cell reference, you can go to the Output sheet, right-click the correct cell and select Copy cell reference (**Fig. 21**).

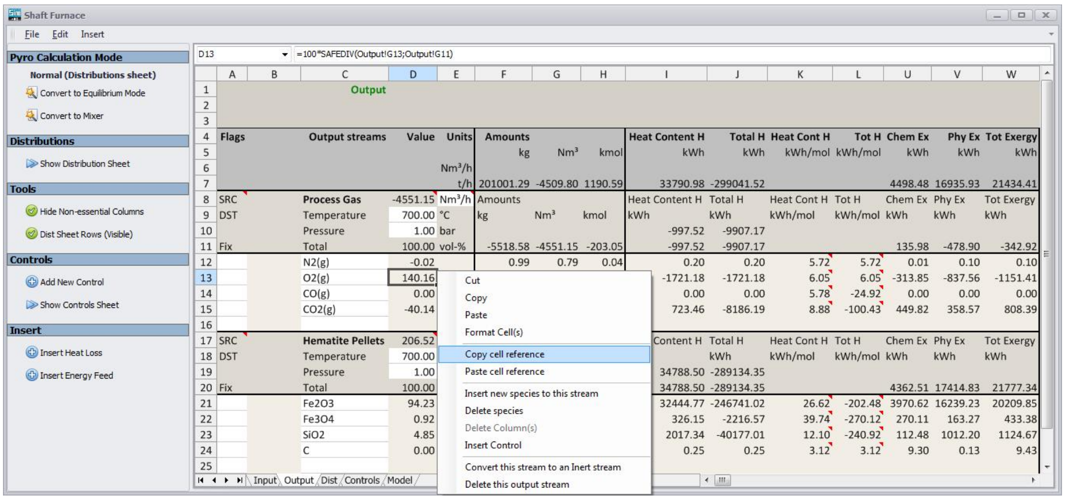


Fig. 21. Copy the cell reference of O2 % in the gas stream.

Then set this cell reference as the control by selecting Paste cell reference for the Measured value of the O2 % control, cell D12 (**Fig. 22**).

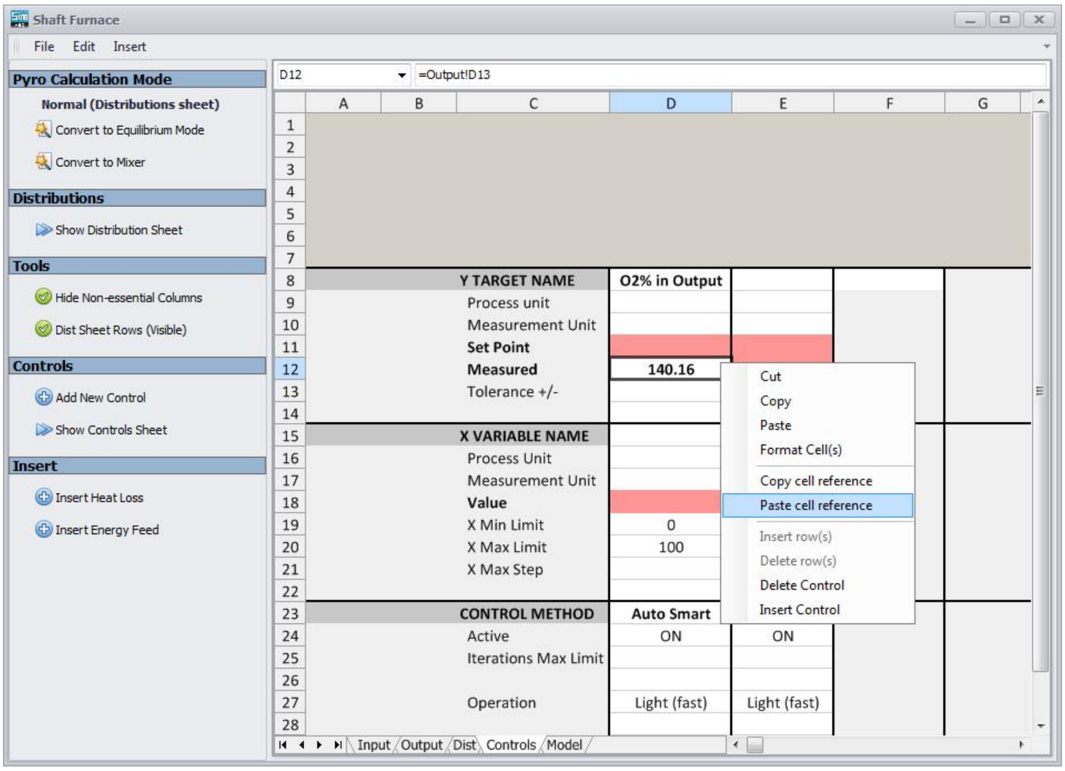


Fig. 22. Set cell reference for the target parameter.

For this target parameter you must assign the Set Point value, which will be the goal that the control tries to reach. In this example, the Set Point value will be 5.00 vol-%. It is also recommended to add the process unit and measurement unit to the control (**Fig. 23**). Having the units in the controls helps to keep track of their operation.

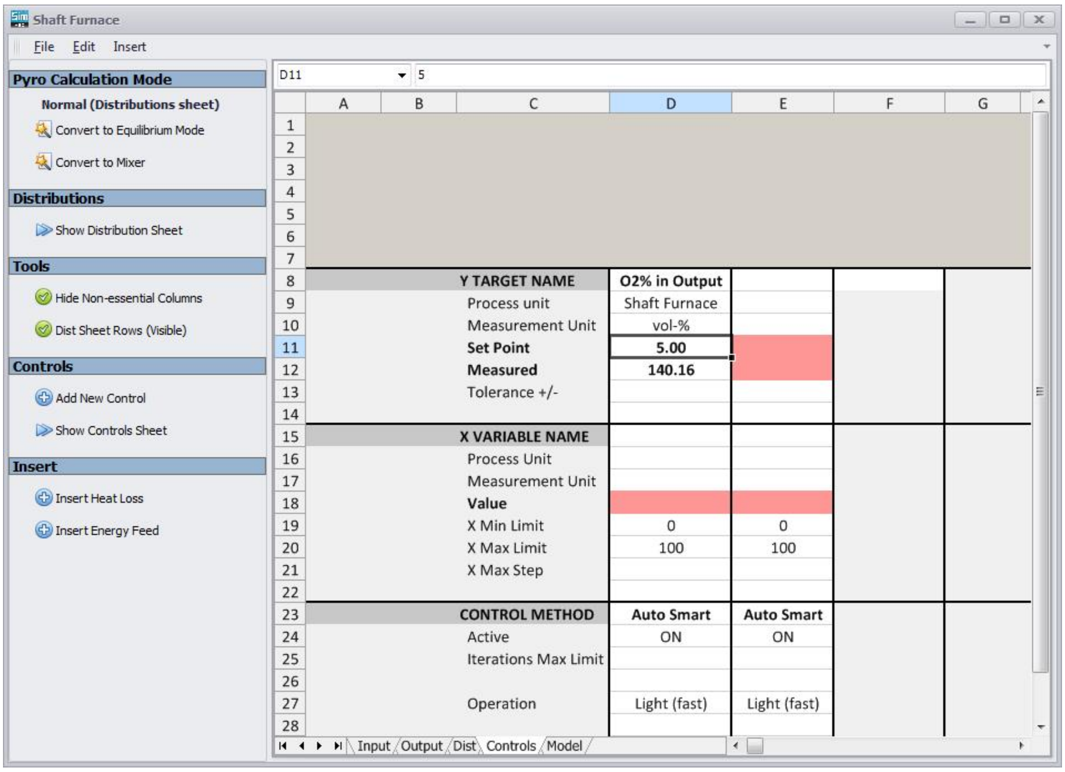


Fig. 23. Assign Set Point value for the control.

Next, set the variable cell reference that will regulate the target parameter. In this example, you can use the total input of the "Air" stream. To set this cell reference, go to the Input sheet and copy the correct cell reference (Input!D22) (**Fig. 24**), and paste the cell reference on the Controls sheet to the Value cell (Controls!D18). Also fill in the process and measurement unit information for the variable parameter (**Fig. 25**).

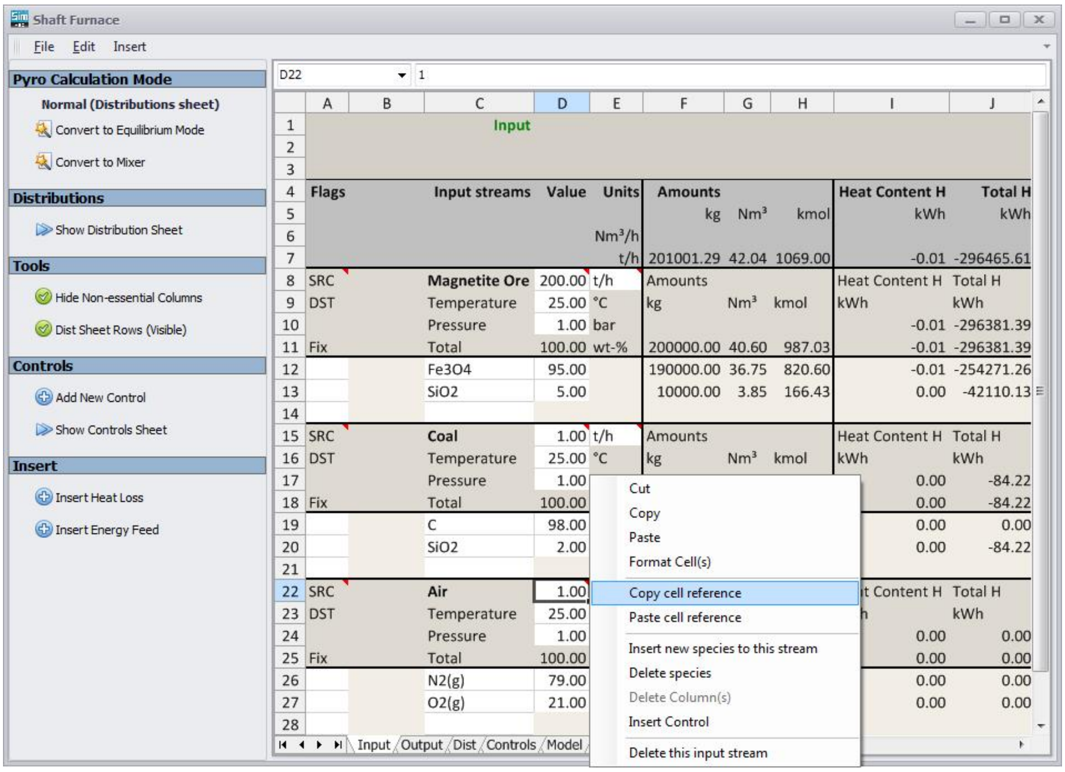


Fig. 24. Copy cell reference of the air feed.

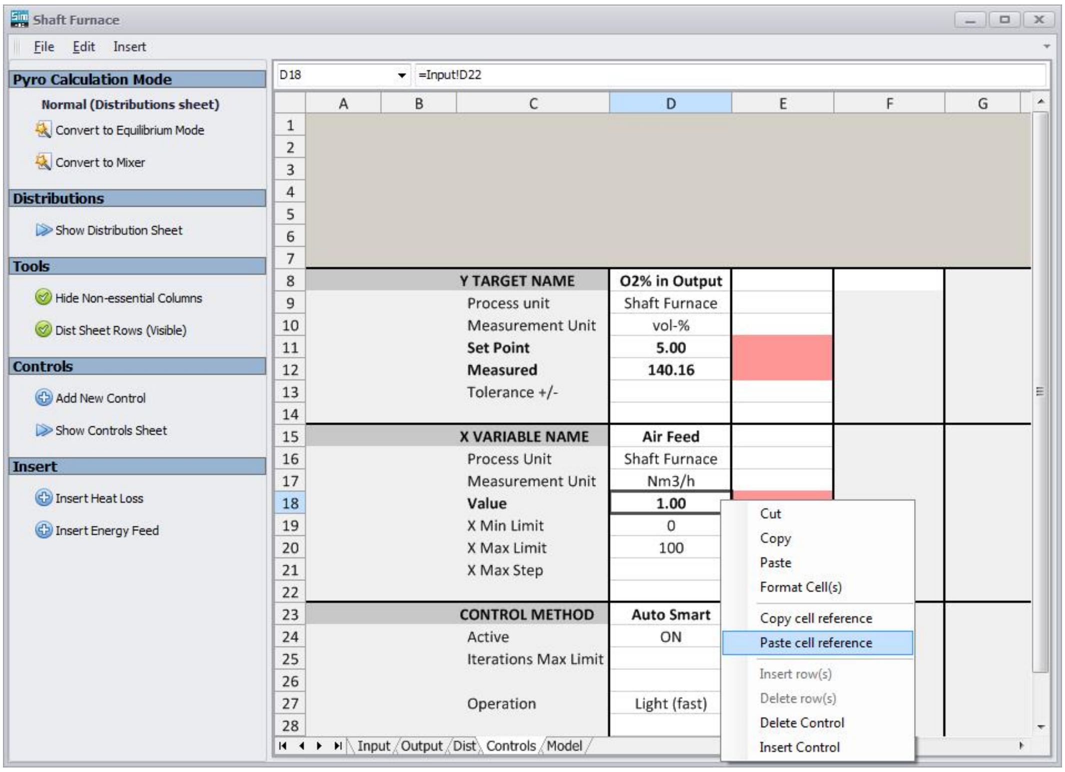


Fig. 25. Set cell reference for the variable parameter.

Finally, it is recommended to adjust the minimum and maximum limits for the variable parameter and to set a tolerance value for the target parameter (**Fig. 26**). After that the O2% control is ready.

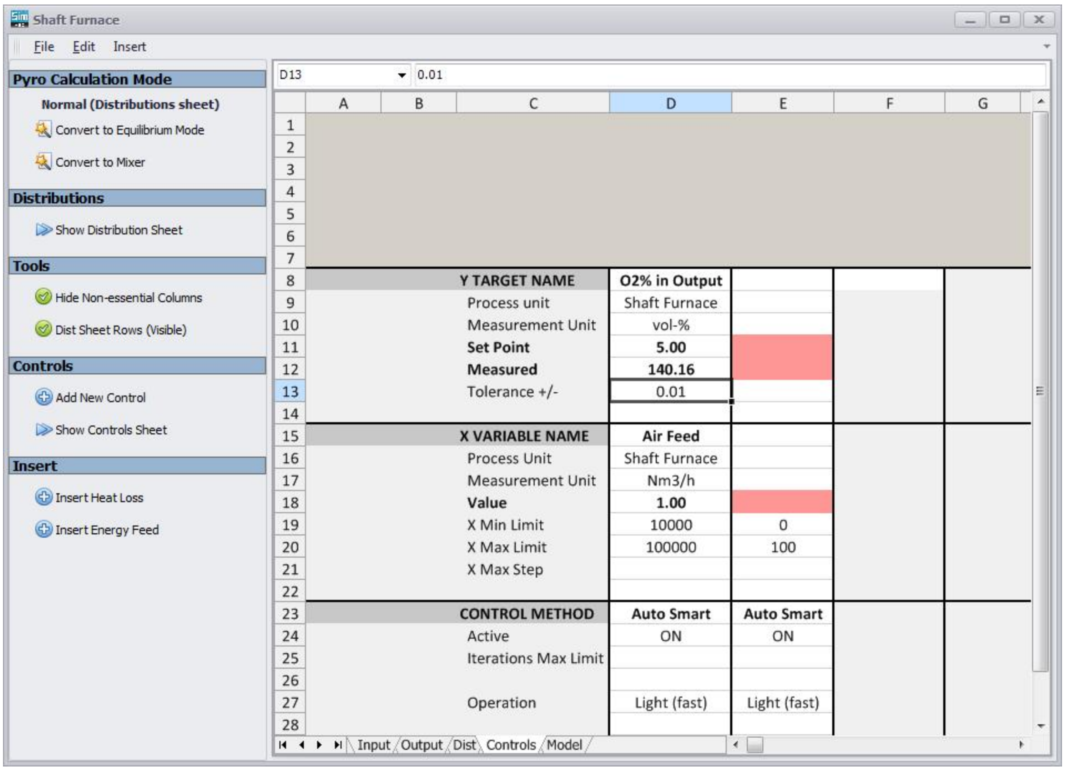


Fig. 26. Variable limits and target tolerance.

The Heat Balance control can be made by following the same steps. First, copy the cell reference for the Total H balance (Dist!J4) (**Fig. 27**).

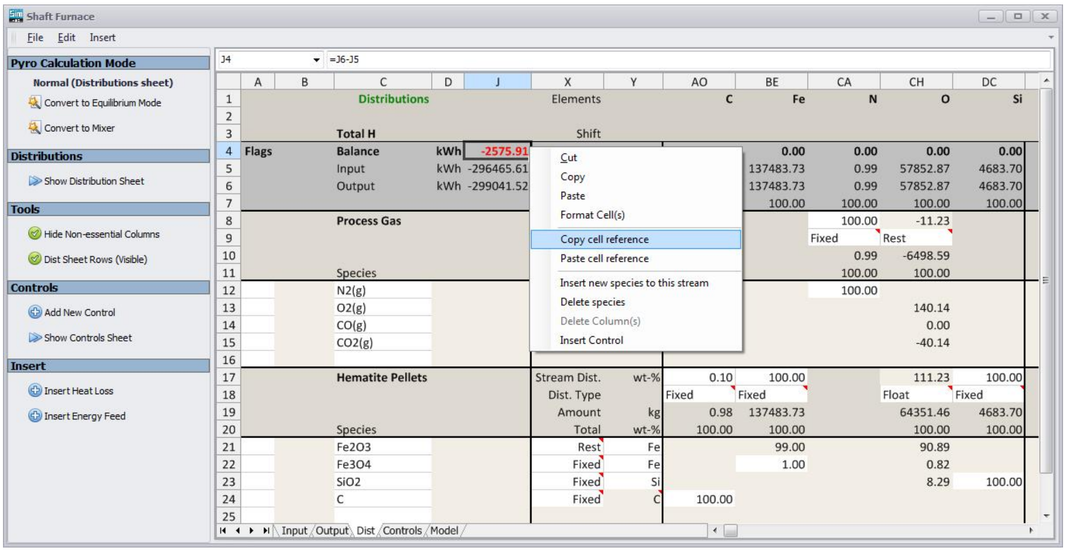


Fig. 27. Copy cell reference of the total enthalpy balance.

Then paste this cell reference to the Measured cell of the Heat Balance control and assign 0.00 as the Set Point (**Fig. 28**).

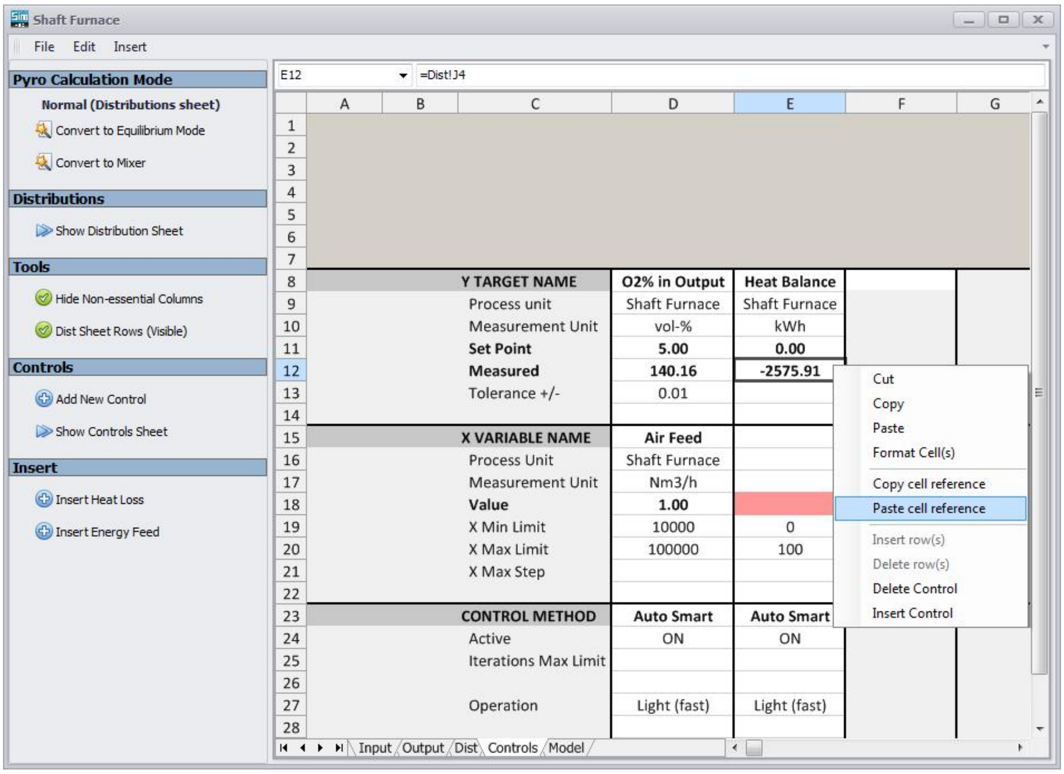


Fig. 28. Set the Total H balance as the target parameter.

The variable to regulate the heat balance can be set as the amount of coal fed into the furnace. Copy the cell reference of the "Coal" stream's total amount (Input!D15) (**Fig. 29**) and paste it to the Value cell of the Heat Balance control (**Fig. 30**).

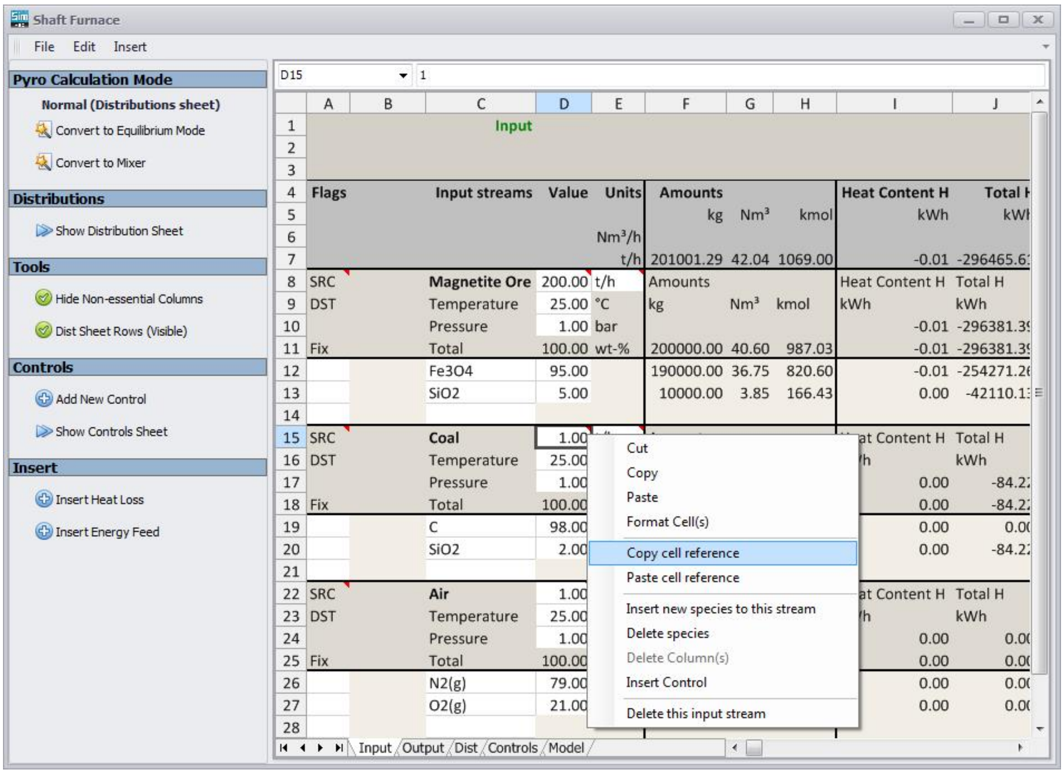


Fig. 29. Copy cell reference of the coal feed.

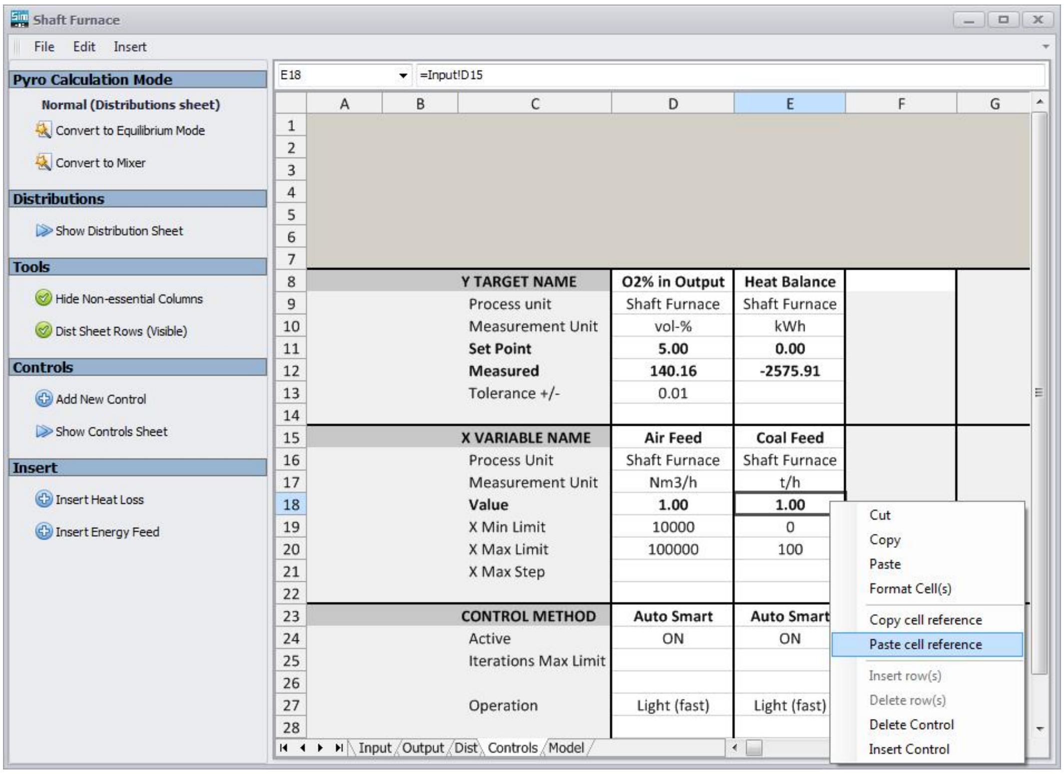


Fig. 30. Set Coal feed as the variable.

To complete the process controls, add a tolerance value for the heat balance and adjust the minimum and maximum limits for the coal feed (**Fig. 31**).

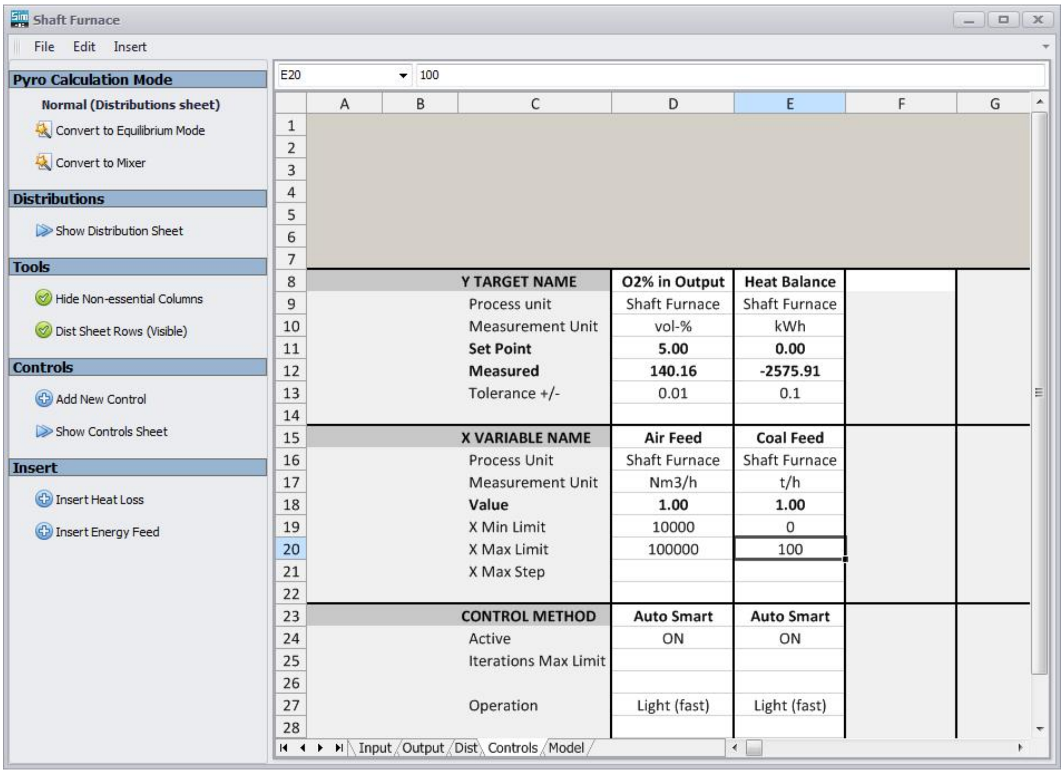


Fig. 31. Completed controls.

42.9. Step 9. Run the Process Model

The process model is now ready and you can start the simulation by pressing the Simulate button at the top bar (**Fig. 32**). Next to the Simulate button you can set the number of iteration rounds. Processes with recycling streams and controls may require several iteration rounds in order to reach steady state.

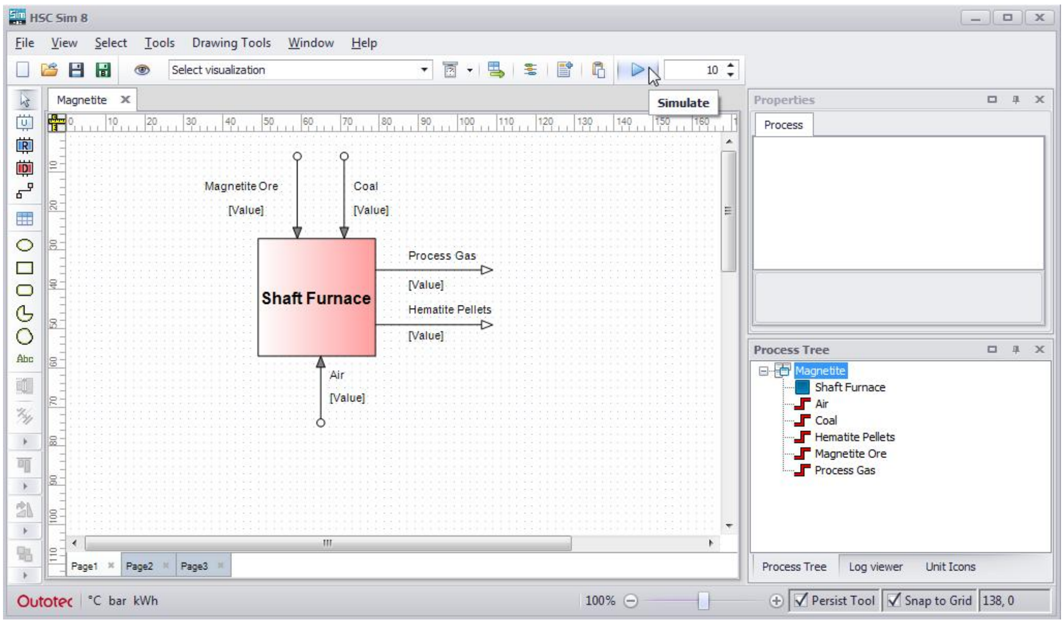


Fig. 32. Simulate the process.

Results of the simulation can be shown on the flowsheet by selecting the Stream Visualization Mode (**Fig. 33**). The selected property in the adjacent dropdown menu is shown in each of the stream value labels (**Fig. 34**).

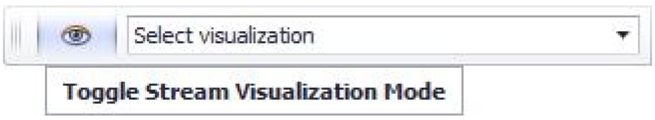


Fig. 33. Stream Visualization.

Visualization can be used with the simulation to study, whether the process reaches steady state. After a few simulation rounds, the value labels should obtain values which no longer change when further simulation rounds are run. It is also recommended to check the controls (**Fig. 35**). They are OK if the Set Point has been reached within the tolerance.

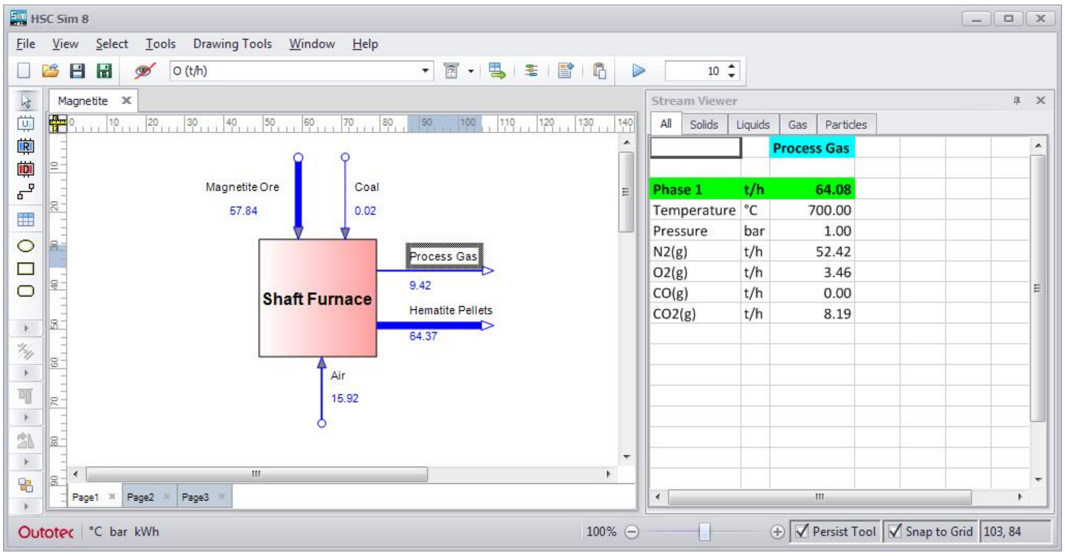


Fig. 34. Element balances and behavior can be seen when element amounts are selected in the visualization. In this screenshot, the diagram shows the behavior of oxygen in the process.

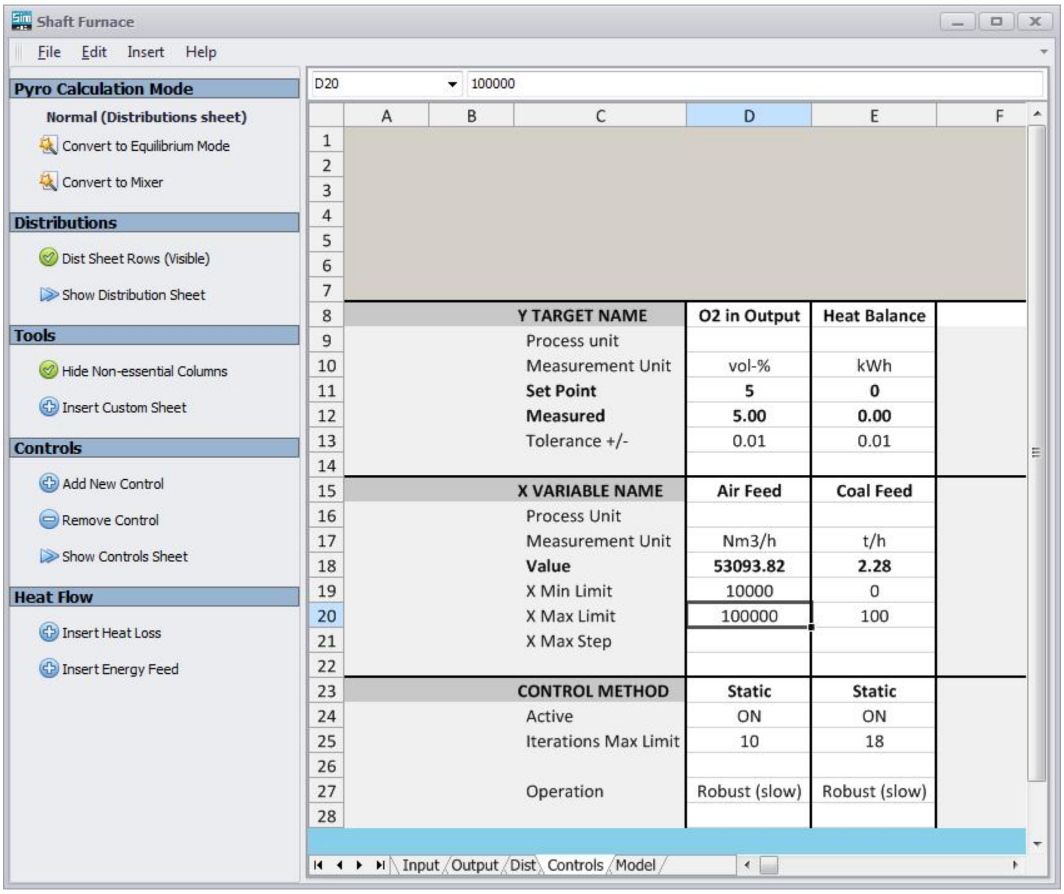
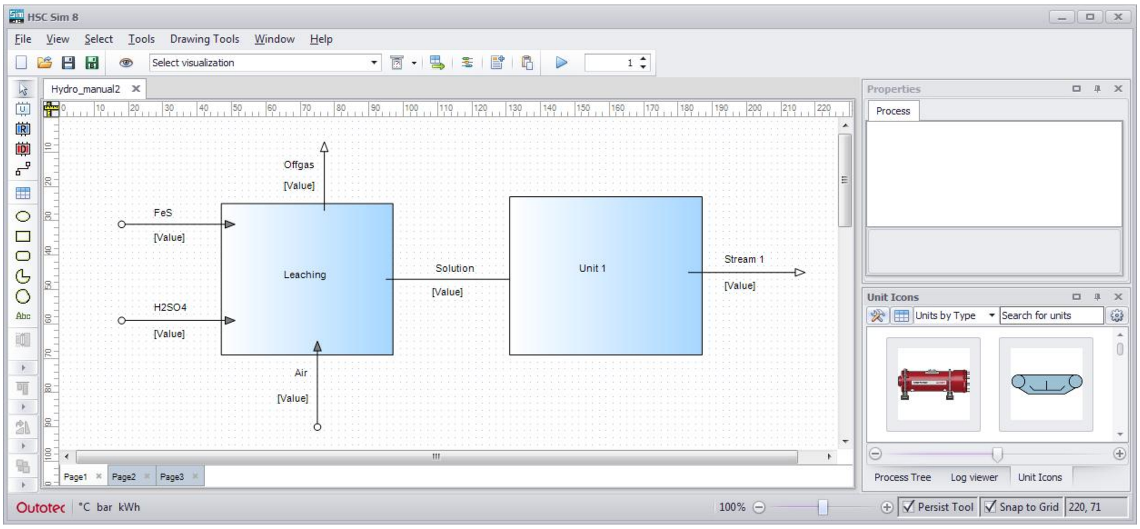


Fig. 35. Controls after simulation.

43. Sim Reactions (Hydro) Unit



The Reactions unit calculates chemical reactions based on unit operations in solid, liquid, and gas systems. This unit was originally made for hydrometallurgical process calculations, but can be used for almost any process, especially those that can be modeled with chemical reactions.

43.1. Steps to Successful Sim Reactions Simulation

It is important to add the necessary information before the simulation can be started. It is good to follow this list while making your Sim Reactions models. Steps 3 to 9 are explained in more detail below.

1. Draw units and streams, see Chapter 40 (section 40.1.)
2. Save Process (see step 8)
3. Create variable list
4. Add reaction equations
5. Specify distributions
6. Set controls
7. Specify raw material amounts
8. Save Process and Save Backup
9. Run process

43.2. Creating a Variable List

A variable list editor is shown in **Fig. 1**. The user should at least add some species to phases in this editor. In this simple (cooler) example, only H_2O has been added to the water phase (row 13) and just the amount has been checked (cell E12), which automatically creates row 17. Default system variables are also shown in rows 3-9 and default phases in rows 10, 12, and 15.

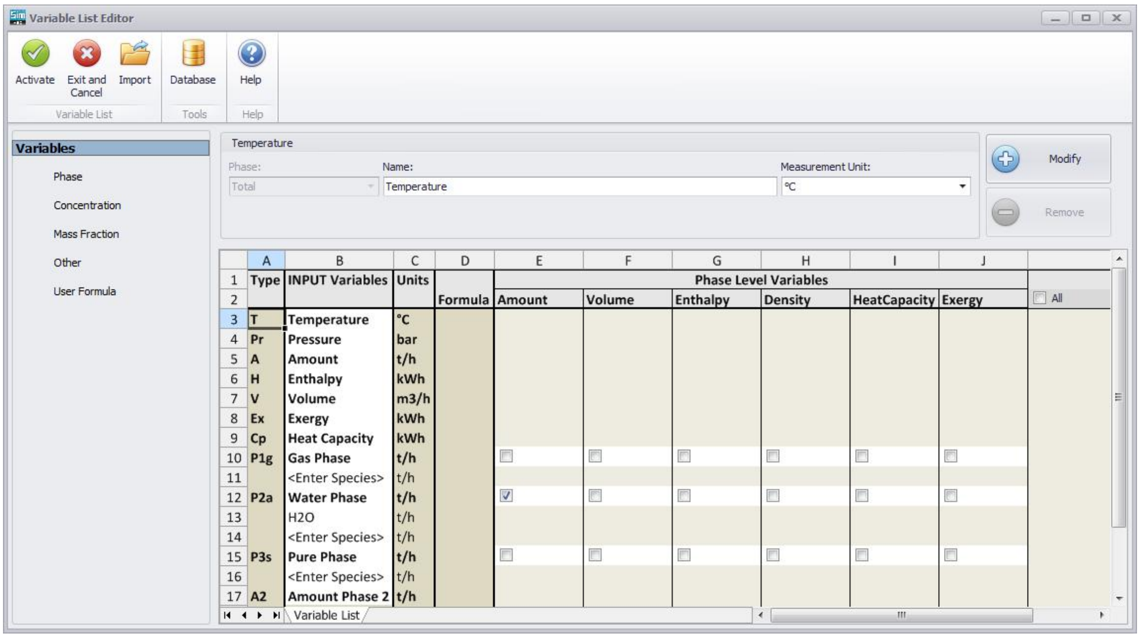


Fig. 1. Variable List Editor where user specifies the variables needed in the simulation.

43.2.1. Filling Variable List Manually

Specify the Species

First you need to specify the species you are using in your calculation. The species can be any combination of elements (like Fe, Ag, O, etc.), solid species ($CaCO_3$, Na_2S, CuS, etc.),

gases (CO_2(g), O_2(g), N_2(g), etc.), or liquids (H_2SO_4(a), $CuSO_4$(a), etc. or Cu(+2a), SO_4(-2a), H(+a), etc.).

Special case: species that are not found in HSC database

If the compound is not found from the HSC database. To use the compound you need to add it to the own database.

Here are instructions what you need to take into account when you add the compound:

The compound needs to have a chemical formula. Molecular weight is calculated from the formula. For mixtures use formula that gives average molecular weight and if you do not know the exact formula use formula that has correct molecular weight.

For example organic compound with average molecular weight of 350 g/mol can be put to the database as: C29(MPEG350).

Note that the last character in brackets defines the phase so it cannot be any of the following characters: a, g, l, s, + or -.

You can add properties to the compound manually, for example enthalpy (kJ/mol), entropy (J/(mol*K)), heat capacity (J/(mol*K)) and density (kg/l). For heat capacity you can fit data for different temperature ranges.

If you know the chemical formula for the compound the enthalpy, entropy and heat capacity values can be estimated with H, S and Cp estimates module.

<u>Example</u>

Organic compound

In copper solvent extraction you have unloaded reagent, loaded reagent and diluent that are not found from the HSC database. You know the density and molecular weight of the compounds. This is one way how you add the compounds to the database.

Type the compound name to the variable list editor. It will open the database editor automatically and copy the compound name to editor if compound is not found from the database.

Type the data for the compound (name and density in units kg/l):

C42H2(unloaded reagent), 0.96
C42Cu(loaded reagent), 1.00
C14(diluent), 0.79

If you know enthalpy, entropy or heat capacity values you can add them for the compounds.

After adding compounds to the database and the densities you can use these organic compounds in your model. The density for the organic phase is calculated automatically from the fed data. The compounds can be used in chemical reactions just like other compounds.

Divide the Species into Phases

Divide the species into meaningful phases, because only this will enable you to calculate phase properties like densities and compositions, **Fig. 1**. Species can be typed manually or they can be imported from the database.

A) Type species formulae manually into <enter species> cells.
B) Go to cell <enter species>, click database button, select species and click Import items button in Database Browser.

Specify the Variables

Phase
Measurement units of different phases

- Gas (Nm^3/h, t/h, kg/h)
- Water, Particles, Organic, Solid (t/h, kg/h)

Default phases are "Gas Phase", "Water Phase", and "Pure Phase". The user can change phase names and add new phases as well using the **Modify** button or delete phases using **Remove**.

Concentrate (Concentration)
Measurement units of different phases

- Gas (wt %, vol % or ppm)
- Water (wt %, g/l or ppm)
- Pure (wt % or ppm)

Mass Fraction
To calculate mass fractions of the Water phase, the user has to give

- A compound which is found in Density Database ($Al_2(SO_4)_3$…$ZnSO_4$)
- A compound (aqueous ion) which is found in the variable list (Al(+3a)…Zn(+2a))

Other
Specify Name (e.g. Solid concentration)
Specify Unit (e.g. g/l)

User Formula
Specify Name (e.g. Solid concentration)
Specify Unit (e.g. g/l)
Insert an Excel-type formula in Column D (e.g. =D13/D7/1000. HSC functions like Molecular weight, MW(“H2O”), can also be used in the formulae)

43.2.2. Importing Ready-Made Variable List

A custom-made variable list allows you to utilize the HSC Sim module in many different types of simulation applications, such as mineralogical, chemical, hydrometallurgical, pyrometallurgical, economic, biological, etc. Only your imagination sets the limits! The custom-made variable list gives a lot of flexibility but the drawback is that the users have to know what they are doing.

This is also the main reason why the specification of the variable list is one of the most important tasks in the new model development stage. It is easy to add/delete/modify the

variable list later on, but it may still be best to try to specify a complete variable list right at the beginning or at least before you start to create the calculation models.

If you have a ready-made variable list available you can use the **Import** button in the Variable list editor and choose the *.xls or *.xlsx file that includes your variable list. Some example files can be found in the HSC Chemistry installation folder …\Flowsheet_Hydro.

43.2.3. Activating Variable List

After filling the variable list manually or importing it, the next thing is to click **Activate**.

43.2.4. Summary of Columns

The meaning of the Input, Output, and Dist sheet columns can be summarized as follows:

Column A - Type: Specifies the row type:

- **T** Temperature
- **Pr** Pressure
- **A** Amount
- **H** Enthalpy
- **V** Volume
- **Ex** Exergy
- **Cp** Heat Capacity
- **P** Phase
- Species
- **D** Density (mass fractions also need to be specified for water phase species)
- **C** Concentration (concentrate)
- **F** Mass Fraction (base species must be specified)
- **O** Other
- **U** User formula

The number section in the row type parameter refers to the phase number. For example: A2 = Amount of phase 2, H3 = enthalpy of phase 3, etc.

Column B - Variable: Specifies the variable name.

Column C - Unit: Specifies the measurement unit. Use the same measurement units within all the process unit models.

Column D - Formula: Specifies the Excel-type cell formula which will automatically be added into model Input and Output sheets in Column D and in all the stream columns. HSC AddIn functions can also be used, e.g. MW("H2O").

The HSC AddIn function =Units ("C";"MJ") will check whether the temperature and energy units are as specified in the formula. The user may change the measurement units only in the variable list editor.

Columns E - Streams: Each stream has a column of its own.

43.3. Adding Reaction Equations to Create Calculation Model

In the reactions unit, the mathematical connection (model) between the Input and Output streams is created using Chemical Reactions Wizard. This model transforms the raw materials into products by using chemical reactions given by the user, see **Fig. 3**.

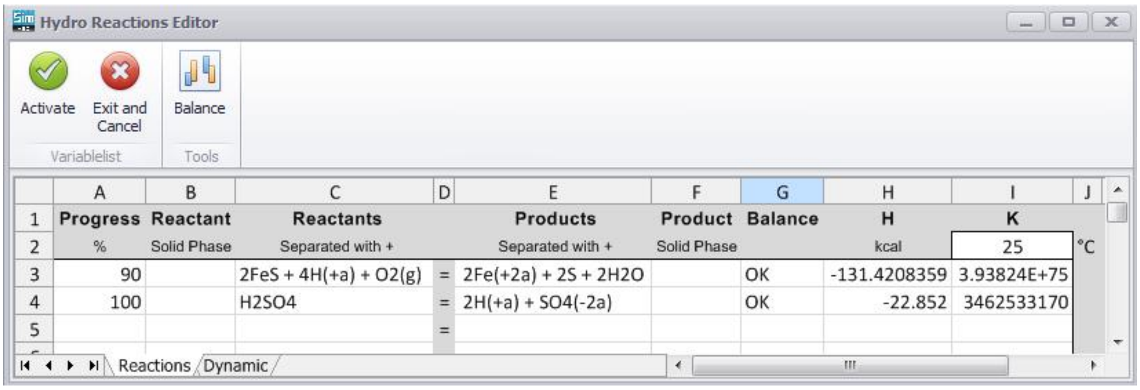


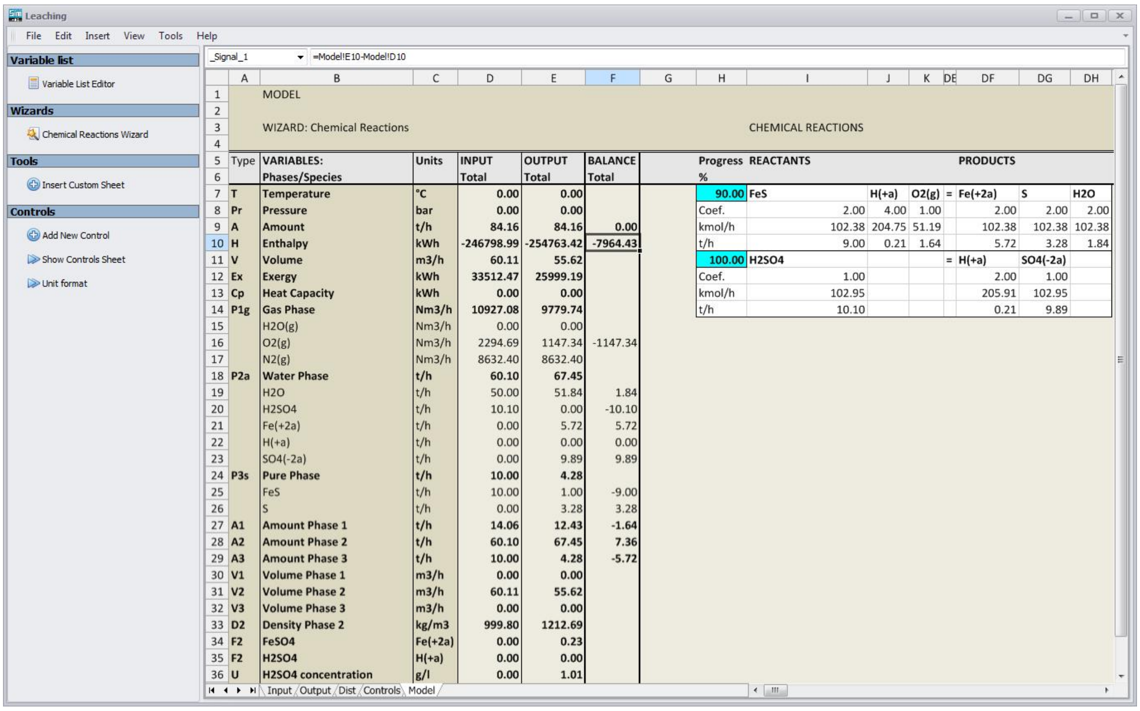
Fig. 2. In Chemical Reactions Wizard the user specifies reaction equations and their progress.

The first step is to enter the reactions that happen in the process unit in the Chemical Reactions Wizard, **Fig. 2**. The species used in the reactions must exist in the variable list.

The first species of each reaction is assumed to be the "raw material" which is consumed in this reaction according to the progress %. For example, FeS is the raw material in reaction 1. You must keep in mind that more than 100% of the raw materials cannot be consumed. The sum of Progress % cannot be more than 100% for the same raw material, although it may be less than 100%. The other species in the reaction equations will automatically be taken into account when a model is created based on the reaction stoichiometry. However, it is still recommended to check whether there are negative amounts on the Model sheet and remove them, for example, by decreasing the Progress %.

The second step is to test the balances by pressing the Balance button. This gives an OK in the Balance column, showing that everything is acceptable. The balance test will also give enthalpy H and equilibrium constant K for the reaction at 25 °C if all the species are found in the active HSC databases. Negative H values mean that heat is released in the reaction, whereas positive values mean that more heat is needed. Large K values (>1) mean that the reaction tends to go to the right and small values (<1) mean that the reaction tends to go to the left in the equilibrium state.

The third step is to **Activate** the reaction equations. After that the reactions can be seen on the model sheet. This sheet contains a list of the reactions with progress percentages. The user may change the Progress % cells (H7 and H11) manually or by using a control, see **Fig. 3.** NB! The species name is **red** if it is not found in the variable list. This will lead to material balance errors since the missing species will not be copied to the output sheet.



	Type	VARIABLES: Phases/Species	Units	INPUT Total	OUTPUT Total	BALANCE Total
7	T	Temperature	°C	0.00	0.00	
8	Pr	Pressure	bar	0.00	0.00	
9	A	Amount	t/h	84.16	84.16	0.00
10	H	Enthalpy	kWh	-246798.99	-254763.42	-7964.43
11	V	Volume	m3/h	60.11	55.62	
12	Ex	Exergy	kWh	33512.47	25999.19	
13	Cp	Heat Capacity	kWh	0.00	0.00	
14	P1g	Gas Phase	Nm3/h	10927.08	9779.74	
15		H2O(g)	Nm3/h	0.00	0.00	
16		O2(g)	Nm3/h	2294.69	1147.34	-1147.34
17		N2(g)	Nm3/h	8632.40	8632.40	
18	P2a	Water Phase	t/h	60.10	67.45	
19		H2O	t/h	50.00	51.84	1.84
20		H2SO4	t/h	10.10	0.00	-10.10
21		Fe(+2a)	t/h	0.00	5.72	5.72
22		H(+a)	t/h	0.00	0.00	0.00
23		SO4(-2a)	t/h	0.00	9.89	9.89
24	P3s	Pure Phase	t/h	10.00	4.28	
25		FeS	t/h	10.00	1.00	-9.00
26		S	t/h	0.00	3.28	3.28
27	A1	Amount Phase 1	t/h	14.06	12.43	-1.64
28	A2	Amount Phase 2	t/h	60.10	67.45	7.36
29	A3	Amount Phase 3	t/h	10.00	4.28	-5.72
30	V1	Volume Phase 1	m3/h	0.00	0.00	
31	V2	Volume Phase 2	m3/h	60.11	55.62	
32	V3	Volume Phase 3	m3/h	0.00	0.00	
33	D2	Density Phase 2	kg/m3	999.80	1212.69	
34	F2	FeSO4	Fe(+2a)	0.00	0.23	
35	F2	H2SO4	H(+a)	0.00	0.00	
36	U	H2SO4 concentration	g/l	0.00	1.01	

Progress %	REACTANTS				PRODUCTS		
90.00	FeS	H(+a)	O2(g)	=	Fe(+2a)	S	H2O
Coef.	2.00	4.00	1.00		2.00	2.00	2.00
kmol/h	102.38	204.75	51.19		102.38	102.38	102.38
t/h	9.00	0.21	1.64		5.72	3.28	1.84
100.00	H2SO4			=	H(+a)	SO4(-2a)	
Coef.	1.00				2.00	1.00	
kmol/h	102.95				205.91	102.95	
t/h	10.10				0.21	9.89	

Fig. 3. Model sheet shows user-defined chemical reactions.

43.3.1. Unit Model Editor - Excel Wizards

Ready-made Excel wizards for some units like **Filter** and **Thickener** were used in HSC7. These wizards are also available in HSC8; however, they will no longer be supported in the future so we recommend users not to use them any more. New dll units can be used for this purpose.

Unit model editor is activated from the **Tools menu** in the main flowsheet window (or right mouse click over any unit). In the editor, the user can choose a unit, double-click the wizard and click OK. The user then specifies the streams and after that the model is ready to be used, see also Chapter 40 (section 40.2.2).

43.4. Distributions

The Dist sheet is filled because the user must divide the products into the output streams. If there is only one output stream then 100% of the products enter this stream. The example in **Fig. 4** shows a distribution where all the gas species enter the Offgas stream (type 100 in cell F14) and all the water and pure species go to the solution phase (type 100 in cells E18 and E24).

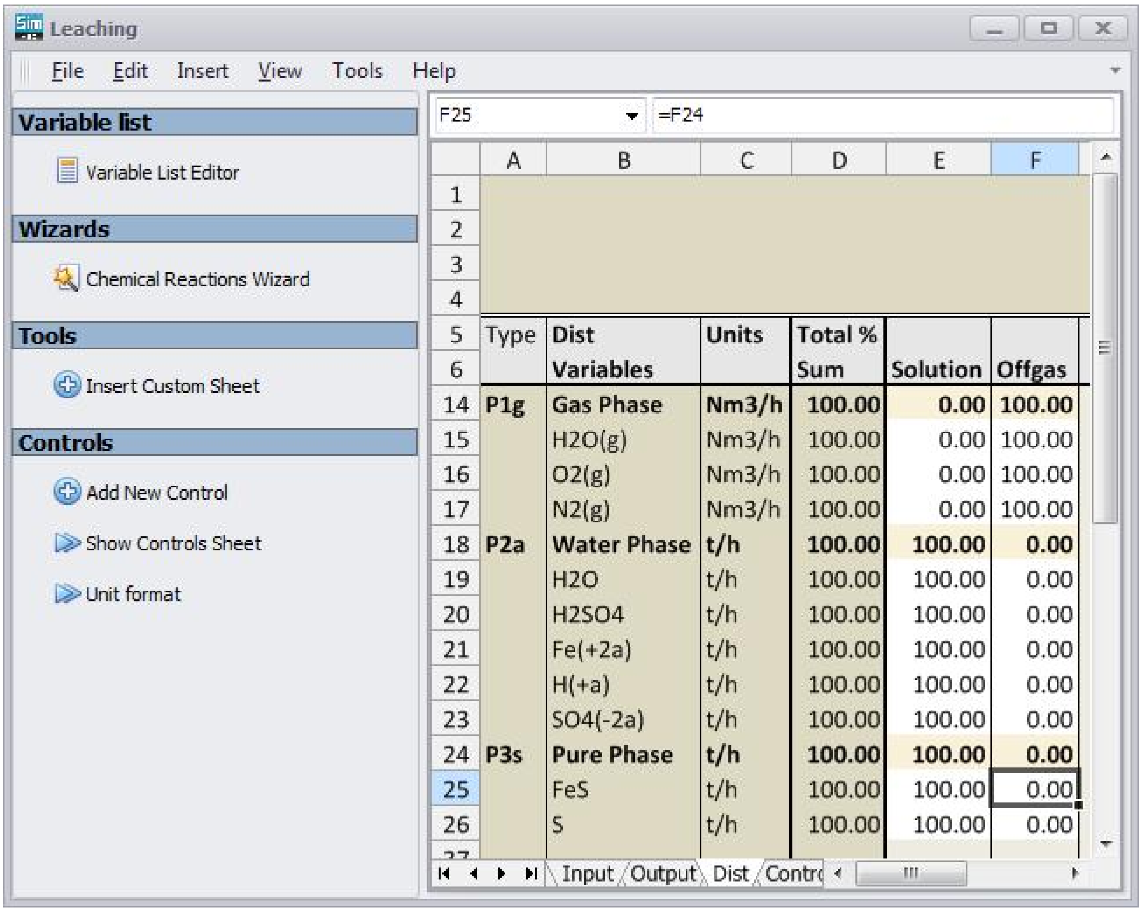


Fig. 4. Dist sheet is usually filled with given distribution percentages.

43.5. Creating Controls

Controls can be added, removed and seen using quick links on the left column, see **Fig. 5**.

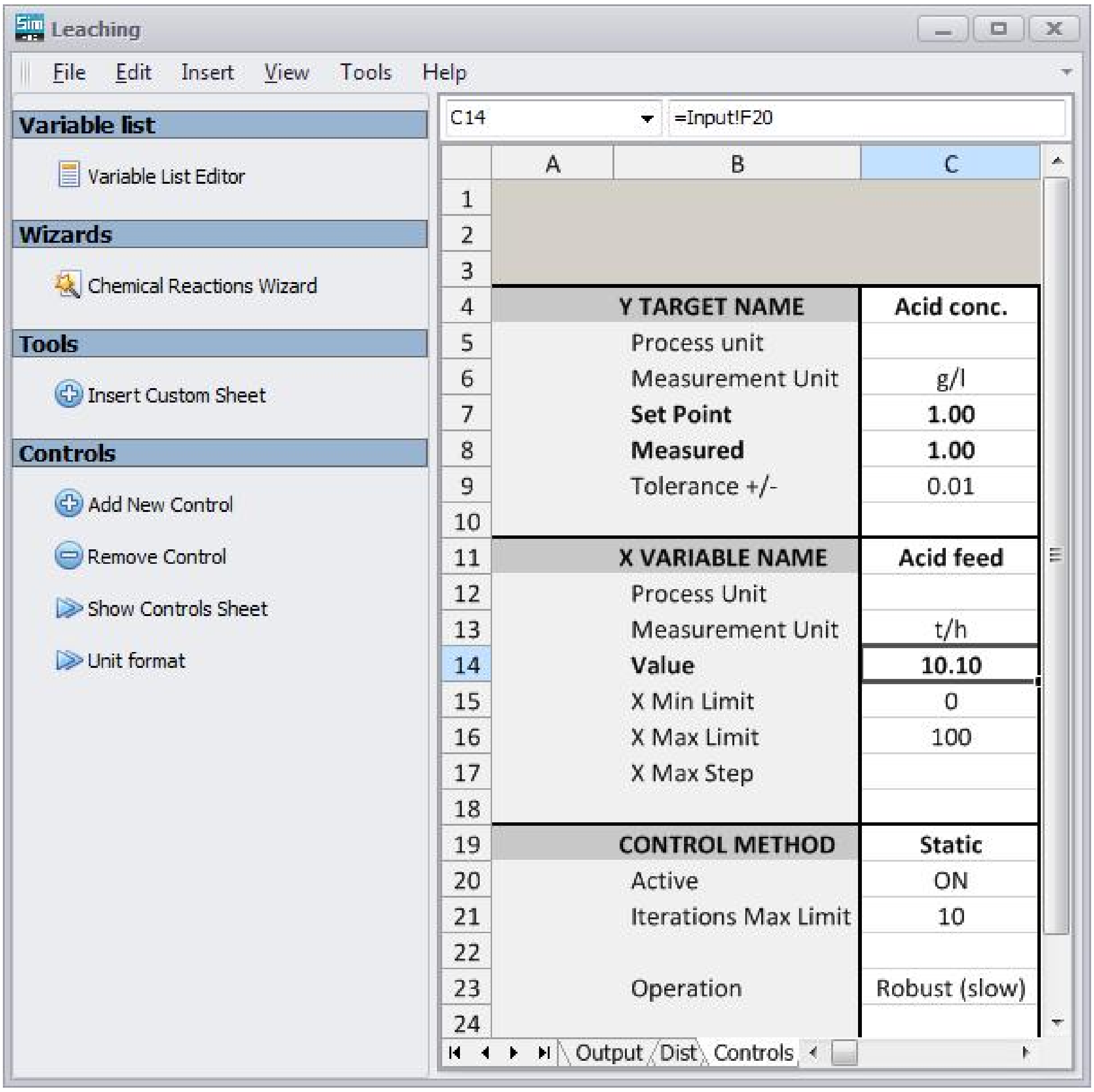


Fig. 5. The calculation model “Controls sheet” with one control.

The HSC Sim Controls sheet makes it possible to create controls that regulate the target parameter cell value using another variable cell value, see **Fig. 5**. In principle, Sim Control works exactly like a real process control. For example, in a real process unit you can assign a set point to the process unit temperature and regulate the temperature by changing the fuel oil feed.

To create a control on the Controls sheet, you have to set at least the set point, the Target cell reference, the Variable cell reference, the limits for the variable, and the tolerance. You can type this information on the Controls sheet using the following procedure:

1. Type the name and the unit of measure in Control sheet cells C4 to C6 (optional).
2. Type Target set value in cell C7.
3. Locate the Target cell from your active unit and right mouse click "Copy cell reference".

4. Go to Control sheet cell C8 and right mouse click "Paste cell reference".

5. Give the tolerance of the calculation in cell C9. When the difference between the Set Point and the Measured value is smaller than the Tolerance, the control is in balance and will not be calculated further.

6. Type the name and the unit of measure in cells C12 and C13 (optional).

7. Locate the Variable cell from your active unit and select "Copy cell reference".

8. Go to Control sheet cell C14 and right mouse click "Paste cell reference".

9. Type **Limit Min** and **Max** in cells C15 and C16; a narrow numerical range speeds up the calculations.

The default **Tolerance** is +/-. A small tolerance increases the calculation time and a large tolerance increases errors. Some 2% of the target value may be a good compromise. The control will not be taken into account if the value is within the tolerance.

Sim Controls have exactly the same **limitations** as real process controls, for example:

- If the target cell does not depend on the variable cell value, the iterations will fail.
- If an external variable cell is used, there may be a long delay before the effect on the target value becomes visible. In these cases a lot of iteration rounds might be needed to reach the set point. This increases the calculation time.

Table 1. Information on the Control sheet.

Row	Name	Description
4	Y Target Name	Name of Y (optional)
5	Process Unit	Unit name (optional)
6	Measurement Unit	Name of the unit of measure (optional)
7	**Set Point**	**Set point of Y (obligatory)**
8	**Measured**	**Y cell reference (obligatory)**
9	**Tolerance +/-**	**Y tolerance (obligatory)**
11	X Variable Name	Name of X (optional)
12	Process Unit	Unit name (optional)
13	Measurement Unit	Name of the unit of measure (optional)
14	**Value**	**X cell reference (obligatory)**
15	**X Min Limit**	**Min limit of the X range (obligatory)**
16	**X Max Limit**	**Max limit of the X range (obligatory)**
17	X Max Step	Maximum X Step (optional, default = empty)
19	Control Method	Iteration method (optional, default = Auto[1])
20	Active	Set control ON/OFF (optional, default = empty = ON)
21	Iterations max limit	Max number of iterations (optional, default = 10)
22	Iterations min limit	Min number of iterations (optional, default = empty)
23	Operation	Control calculation operation (optional, default = Light[2])

[1]**Auto** (Solves the control with information on rows 20 - 23), **Auto Smart** (Same as Auto except changes X Max Step and Iterations max limit when needed), **PID** (not in use, will be added to HSC8 version).

[2]**Light** (Solves the control with modified tangent method, fast), **Robust** (Solves the control with modified Newton method, slow), **Simple direct** (Increases X value when Measured value is too small. The step used can be specified in X max step.), **Simple reverse** (Decreases X value when Measured value is too small. The step used can be specified in X max step.).

43.5.1. Internal and External Controls

1. Internal control in which the target and variable cells exist in the same process unit (FAST).

2. External control in which the target and variable cells exist in different process units (SLOW).

Calculation of an internal control is fast because only one unit is calculated. Usually you can create a large number of **internal controls** in a process without a dramatic drop in calculation speed because they do not increase the number of calculation rounds of the process.

Calculation of an external control might take more time because material must be recirculated within the whole process several times to reach a stable target value. Usually only a few **external controls** can be used in one process without a considerable decrease in the calculation speed because external controls might multiply the calculation rounds of the process.

Sometimes it is easier to set controls using additional sheets, where some calculations may be done. You can insert new sheet using left column quick link Insert Custom Sheet or by using menu Insert…Sheet.

43.5.2. Advices When Using Controls

- It is recommended to moderate large changes of the variable with the use of **X Max Step** when using external controls with slow responses.
- If you want to keep some concentration lower than a set point (8 g/l), change the bleed stream amount (valve 0 - 100%). Please use an external control since the bleed amount will not change the concentration unless the whole process is calculated. This is possible when the bleed and concentration cells are in different units.
- The **RecoveryX** add-in function cannot be used in the Target cell, because it is recalculated only after all the calculation rounds have been completed.
- The large number of thermochemical add-in functions (**StreamH**, StreamS, etc.) may reduce the calculation speed if the argument value changes in each control iteration round, because the data search from the H, S, and Cp database takes time. Use these add-in functions only when needed.

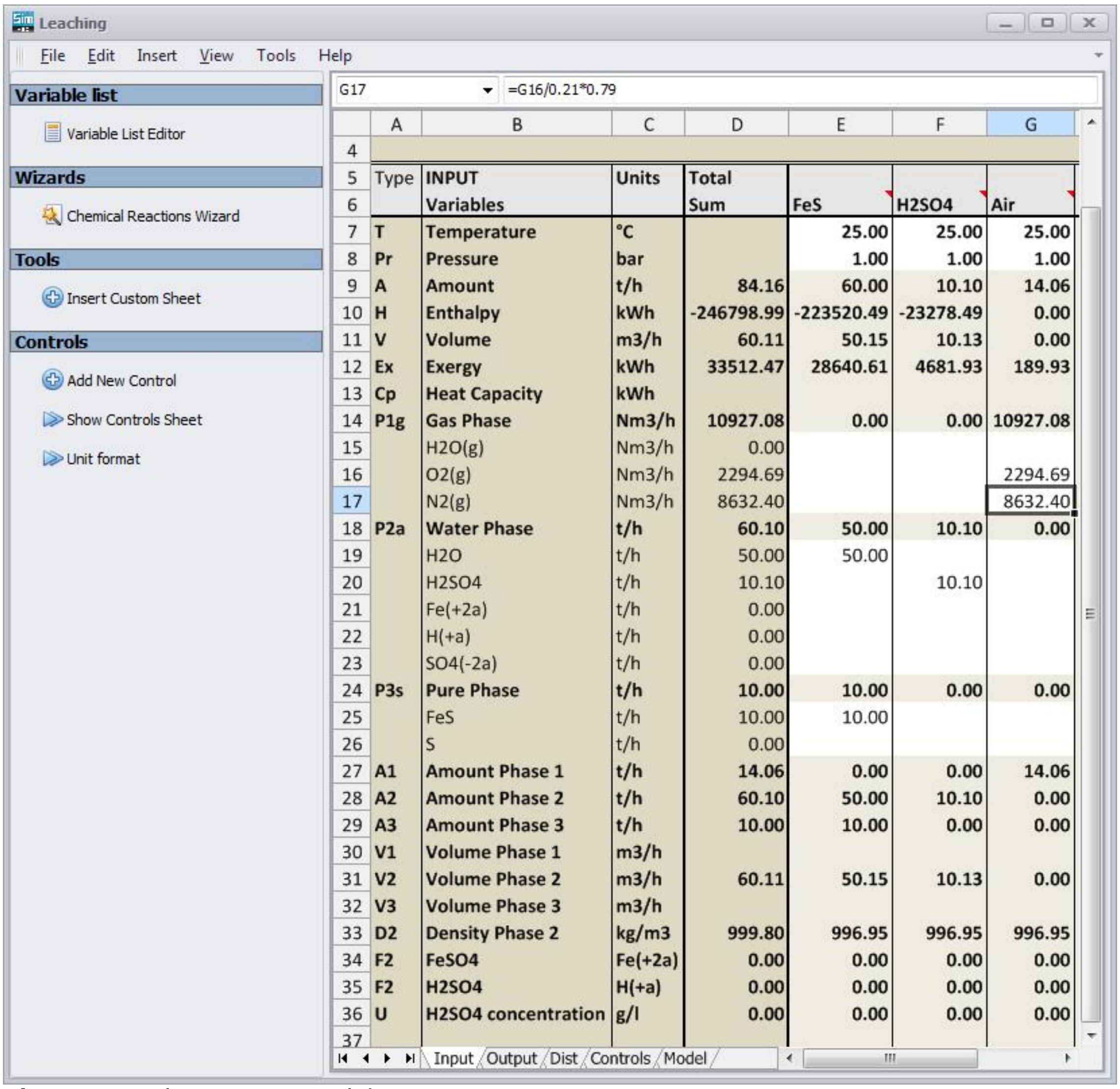
43.6. Adding Raw Materials

In both input and output sheets if the cells are white it means that the user can edit them.

43.6.1. Input Sheet

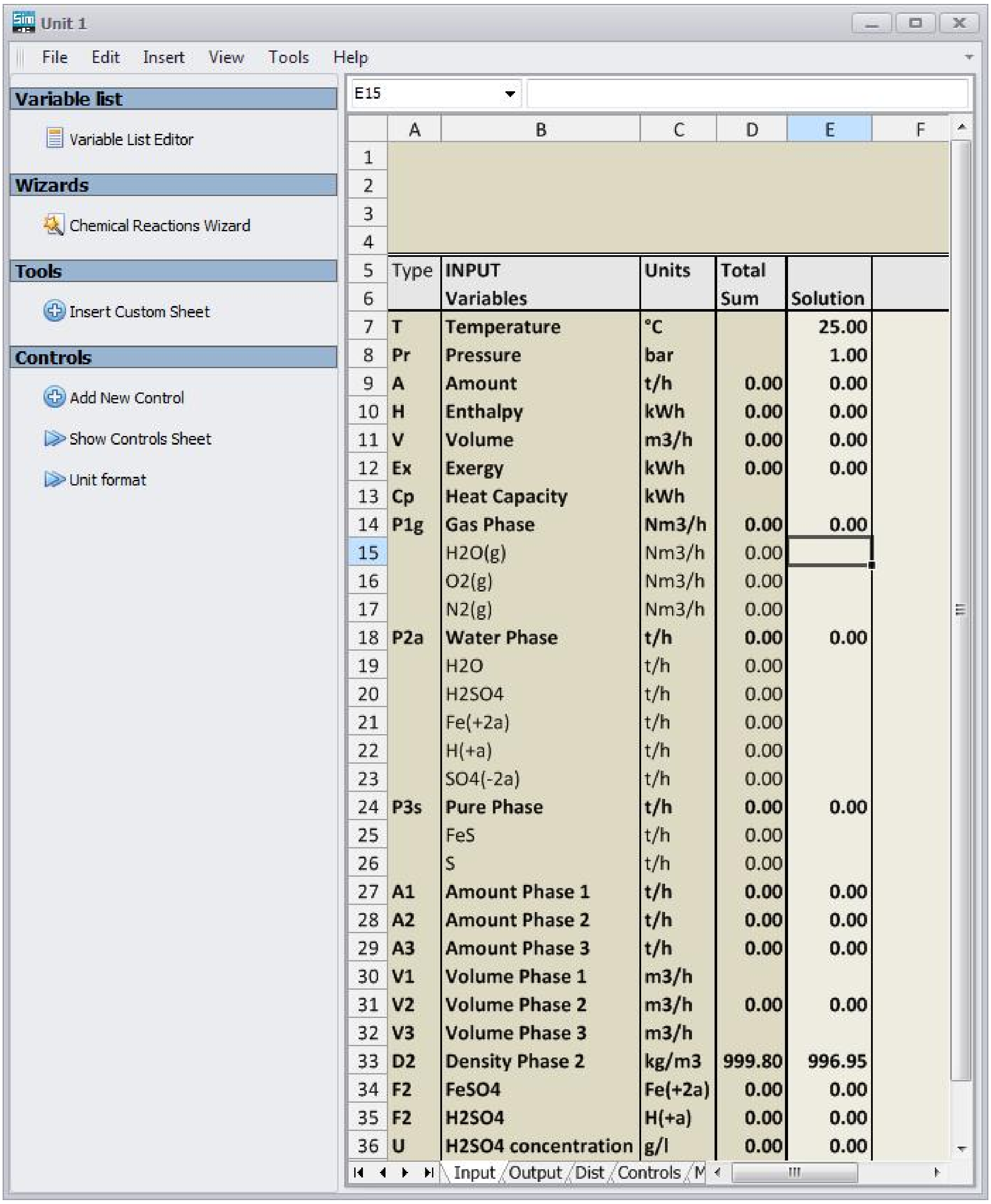
In the input sheet, temperature row 7, pressure row 8, and the raw material amounts are given. In the example in **Fig. 6,** the amount of H_2O and FeS is known and the O_2(g) and N_2(g) amounts are calculated using equations, whereas the H_2SO_4 amount is calculated using the control. The user can give an initial guess of the sulfuric acid value in cell F20 or it can also be empty before the simulation is started.

If the flowsheet contains more than one unit and the units are connected, intermediate stream properties cannot be edited since these values are calculated, see **Fig. 7**.



	A	B	C	D	E	F	G
4							
5	Type	INPUT	Units	Total			
6		Variables		Sum	FeS	H2SO4	Air
7	T	Temperature	°C		25.00	25.00	25.00
8	Pr	Pressure	bar		1.00	1.00	1.00
9	A	Amount	t/h	84.16	60.00	10.10	14.06
10	H	Enthalpy	kWh	-246798.99	-223520.49	-23278.49	0.00
11	V	Volume	m3/h	60.11	50.15	10.13	0.00
12	Ex	Exergy	kWh	33512.47	28640.61	4681.93	189.93
13	Cp	Heat Capacity	kWh				
14	P1g	Gas Phase	Nm3/h	10927.08	0.00	0.00	10927.08
15		H2O(g)	Nm3/h	0.00			
16		O2(g)	Nm3/h	2294.69			2294.69
17		N2(g)	Nm3/h	8632.40			8632.40
18	P2a	Water Phase	t/h	60.10	50.00	10.10	0.00
19		H2O	t/h	50.00	50.00		
20		H2SO4	t/h	10.10		10.10	
21		Fe(+2a)	t/h	0.00			
22		H(+a)	t/h	0.00			
23		SO4(-2a)	t/h	0.00			
24	P3s	Pure Phase	t/h	10.00	10.00	0.00	0.00
25		FeS	t/h	10.00	10.00		
26		S	t/h	0.00			
27	A1	Amount Phase 1	t/h	14.06	0.00	0.00	14.06
28	A2	Amount Phase 2	t/h	60.10	50.00	10.10	0.00
29	A3	Amount Phase 3	t/h	10.00	10.00	0.00	0.00
30	V1	Volume Phase 1	m3/h				
31	V2	Volume Phase 2	m3/h	60.11	50.15	10.13	0.00
32	V3	Volume Phase 3	m3/h				
33	D2	Density Phase 2	kg/m3	999.80	996.95	996.95	996.95
34	F2	FeSO4	Fe(+2a)	0.00	0.00	0.00	0.00
35	F2	H2SO4	H(+a)	0.00	0.00	0.00	0.00
36	U	H2SO4 concentration	g/l	0.00	0.00	0.00	0.00
37							

Fig. 6. Input sheet, raw material amounts.

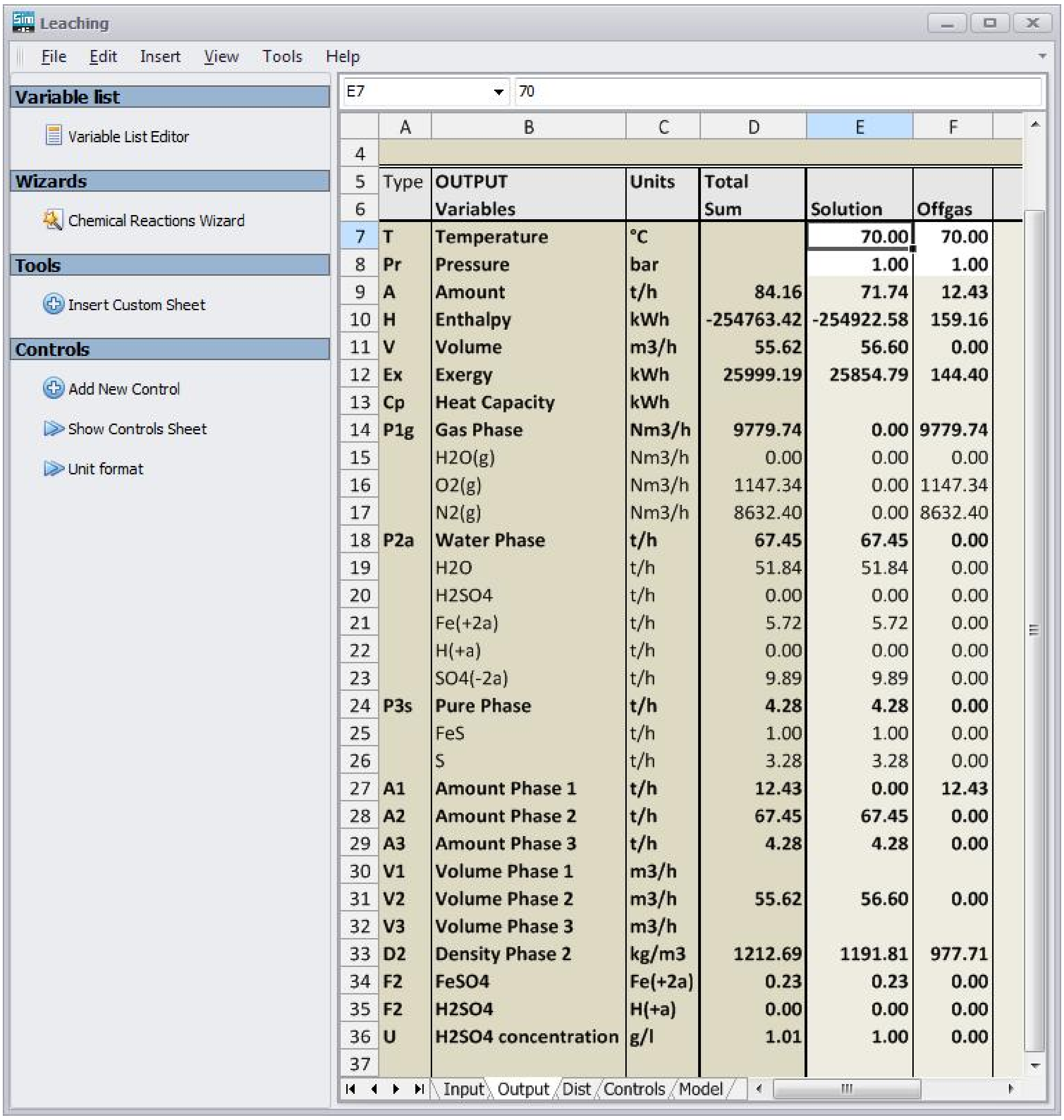


	A	B	C	D	E	F
1						
2						
3						
4						
5	Type	INPUT	Units	Total		
6		Variables		Sum	Solution	
7	T	Temperature	°C		25.00	
8	Pr	Pressure	bar		1.00	
9	A	Amount	t/h	0.00	0.00	
10	H	Enthalpy	kWh	0.00	0.00	
11	V	Volume	m3/h	0.00	0.00	
12	Ex	Exergy	kWh	0.00	0.00	
13	Cp	Heat Capacity	kWh			
14	P1g	Gas Phase	Nm3/h	0.00	0.00	
15		H2O(g)	Nm3/h	0.00		
16		O2(g)	Nm3/h	0.00		
17		N2(g)	Nm3/h	0.00		
18	P2a	Water Phase	t/h	0.00	0.00	
19		H2O	t/h	0.00		
20		H2SO4	t/h	0.00		
21		Fe(+2a)	t/h	0.00		
22		H(+a)	t/h	0.00		
23		SO4(-2a)	t/h	0.00		
24	P3s	Pure Phase	t/h	0.00	0.00	
25		FeS	t/h	0.00		
26		S	t/h	0.00		
27	A1	Amount Phase 1	t/h	0.00	0.00	
28	A2	Amount Phase 2	t/h	0.00	0.00	
29	A3	Amount Phase 3	t/h	0.00	0.00	
30	V1	Volume Phase 1	m3/h			
31	V2	Volume Phase 2	m3/h	0.00	0.00	
32	V3	Volume Phase 3	m3/h			
33	D2	Density Phase 2	kg/m3	999.80	996.95	
34	F2	FeSO4	Fe(+2a)	0.00	0.00	
35	F2	H2SO4	H(+a)	0.00	0.00	
36	U	H2SO4 concentration	g/l	0.00	0.00	

Fig. 7. Input streams of the second unit cannot be edited.

43.6.2. Output Sheet

In the output sheet, temperature row 7 and pressure row 8 are given, see **Fig. 8**. Values in the output sheet are calculated according to the settings in the Dist and Model sheets.



	A	B	C	D	E	F
4						
5	Type	OUTPUT	Units	Total		
6		Variables		Sum	Solution	Offgas
7	T	Temperature	°C		70.00	70.00
8	Pr	Pressure	bar		1.00	1.00
9	A	Amount	t/h	84.16	71.74	12.43
10	H	Enthalpy	kWh	-254763.42	-254922.58	159.16
11	V	Volume	m3/h	55.62	56.60	0.00
12	Ex	Exergy	kWh	25999.19	25854.79	144.40
13	Cp	Heat Capacity	kWh			
14	P1g	Gas Phase	Nm3/h	9779.74	0.00	9779.74
15		H2O(g)	Nm3/h	0.00	0.00	0.00
16		O2(g)	Nm3/h	1147.34	0.00	1147.34
17		N2(g)	Nm3/h	8632.40	0.00	8632.40
18	P2a	Water Phase	t/h	67.45	67.45	0.00
19		H2O	t/h	51.84	51.84	0.00
20		H2SO4	t/h	0.00	0.00	0.00
21		Fe(+2a)	t/h	5.72	5.72	0.00
22		H(+a)	t/h	0.00	0.00	0.00
23		SO4(-2a)	t/h	9.89	9.89	0.00
24	P3s	Pure Phase	t/h	4.28	4.28	0.00
25		FeS	t/h	1.00	1.00	0.00
26		S	t/h	3.28	3.28	0.00
27	A1	Amount Phase 1	t/h	12.43	0.00	12.43
28	A2	Amount Phase 2	t/h	67.45	67.45	0.00
29	A3	Amount Phase 3	t/h	4.28	4.28	0.00
30	V1	Volume Phase 1	m3/h			
31	V2	Volume Phase 2	m3/h	55.62	56.60	0.00
32	V3	Volume Phase 3	m3/h			
33	D2	Density Phase 2	kg/m3	1212.69	1191.81	977.71
34	F2	FeSO4	Fe(+2a)	0.23	0.23	0.00
35	F2	H2SO4	H(+a)	0.00	0.00	0.00
36	U	H2SO4 concentration	g/l	1.01	1.00	0.00
37						

Fig. 8. Output sheet, temperature and pressure of the streams can be changed.

43.7. Save and Run simulation and visualize results

It is good to Save Process and Backup often. It is good habit to save process after each step. Remember to save at least before starting the simulation, see **Fig. 9** and **Fig. 10**. There are many ways to visualize the simulation results, see **Fig. 11** and Chapter 40 (section 40.3.).

Fig. 9. Save Process and Save Backups icons.

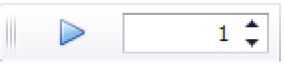


Fig. 10. Run simulation and give iteration rounds to calculations.

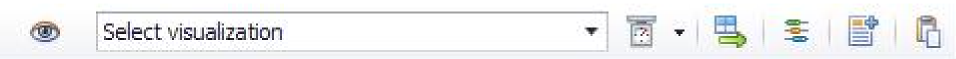


Fig. 11. Visualize results and change units, add stream tables, visualize stream connections, add header or copy flowsheet to clipboard.

Research Center, Pori / Petri Kobylin, Tuukka Kotiranta

44. Sim Reactions Example

44.1. General

This example contains instructions on how to create a simple leaching reactor model where 10 t/h of FeS is leached with acid (H_2SO_4) and air at 70 °C. The water feed is 50 t/h and the FeS leaching efficiency is 90 %, oxygen efficiency is 50 %, and the acid concentration in the product is 1 g/l.

The reactor is cooled with cooling coils. The cooling water input temperature is 25 °C and output temperature 60 °C.

You should keep in mind that streams are put into the input and output sheets in the same order as you have drawn them. This means that when you make a new model the streams might be in a different column than explained here.

The example files can be found from the HSC Chemistry installation folder …Flowsheet_Hydro\Hydro_example3\Hydro_example3.Sim8. This example describes the creation of the flowsheet in detail with references to the Sim Flowsheet manual.

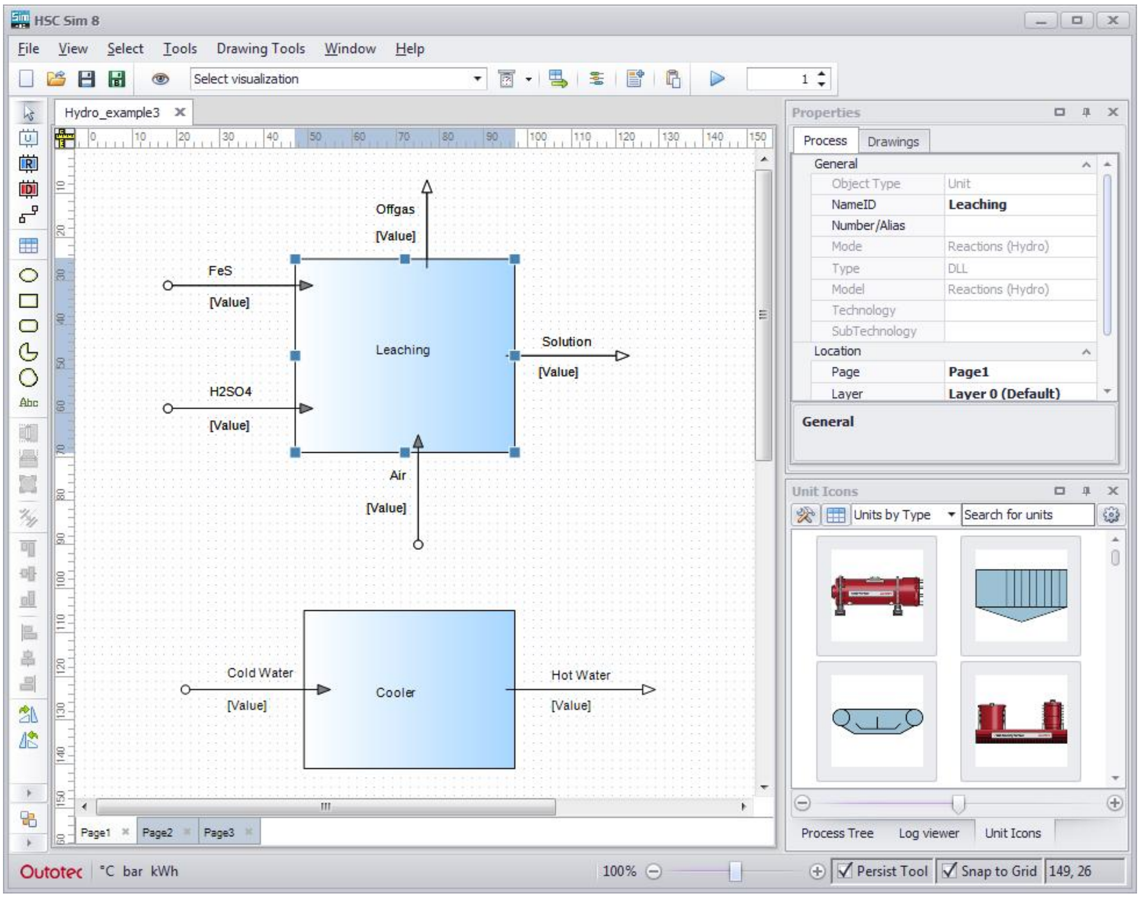


Fig. 1. Sim Reactions Example flowsheet.

44.2. Steps to Successful Sim Reactions Simulation

1. Draw units and streams
2. Save process and save backup
3. Create variable list
4. Add reaction equations
5. Specify distributions
6. Set controls
7. Specify raw material amounts
8. Save process
9. Run process

44.2.1. Drawing a Flowsheet, See Chapter 40 (section 40.1.)

- Draw Reactions **units** (blue).
- Draw input and output **streams**. Left mouse click to start and make corners and double-click to end the stream. For editing the stream afterwards, see section 40.1.2.
- Name the units and streams, see **Fig. 1** and Chapter 40 (section 40.1.3.).
- Check that the source and destination for the streams are correct.

44.2.2. Setting the Variable List, See Chapter 43 (section 43.2.)

A) Import Ready-Made Variable List

In this example two **variable lists** can be used. You can add the lists to the model by double-clicking the unit and clicking Variable List Editor (or in Excel editor, Tools menu and Variable List Editor) and by pressing Import…\Flowsheet_Hydro\Hydro_example3\. For the **Leaching unit** we choose Leaching.xlsx and for the **Cooler unit** Cooler.xlsx, see **Fig. 2** and **Fig. 3**. It is also possible to use Leaching.xlsx list for the Cooler unit but not vice versa.

B) Fill Variable List Manually

You can also fill in the variable lists manually, see **Fig. 2** and **Fig. 3,** or Chapter 43. Use Nm3/h unit for the Gas Phase. You need to give the mass fractions of the water phase otherwise density cannot be calculated (see rows 33-34 in **Fig. 2**). Since H_2SO_4 concentration in g/l is not in the list, you need to create a User Formula (U) in the Variable List Editor.

- Choose User formula and give it a name (H_2SO_4 concentration) and measure unit (g/l).
- Make the formula in column D, see **Fig. 2**. In the example above, the formula in cell D35 is D19/MW(“H”)/2*MW(“H2SO4”)/D30*1000, which means that mass of H_2SO_4 is calculated from the amount of H(+a) ions in moles (see equation in **Fig. 4**) divided by the water phase volume. The result is multiplied by 1000 to obtain the unit grams of H_2SO_4 per liter of solution.
- The User formula is copied automatically to all the Input and Output streams of each unit when Activate is clicked. NB! The equation is changed in the Variable List Editor to “=SAFEDIV(SAFEDIV(D19;MW("H"))/2*MW("H2SO4");D30)*1000” (with equation SAFEDIV HSC8 Sim sets 0/0 = 0).

When modifying the variable list, remember that columns A to D are automatically synchronized, which means that any changes are automatically copied to all the streams.

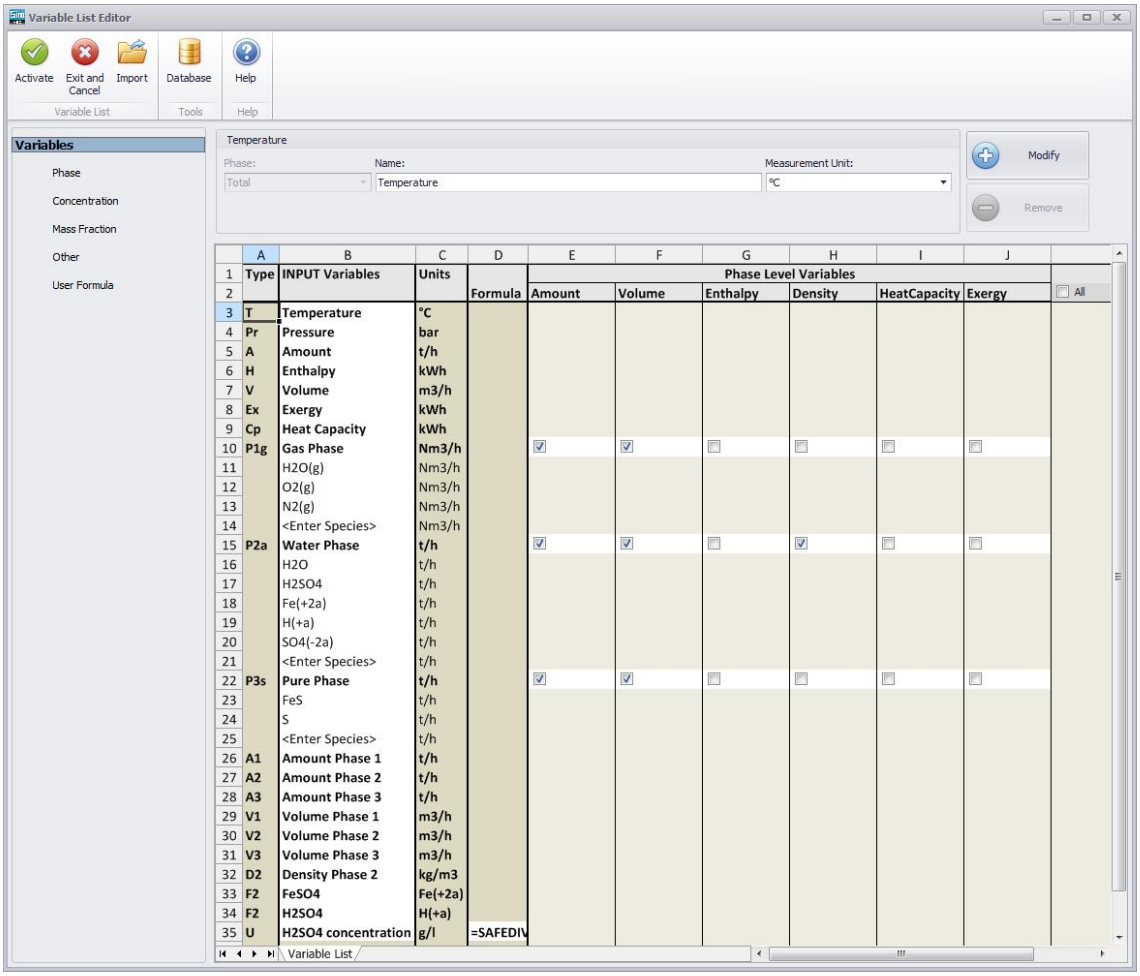


Fig. 2. Variable list of the Leaching unit.

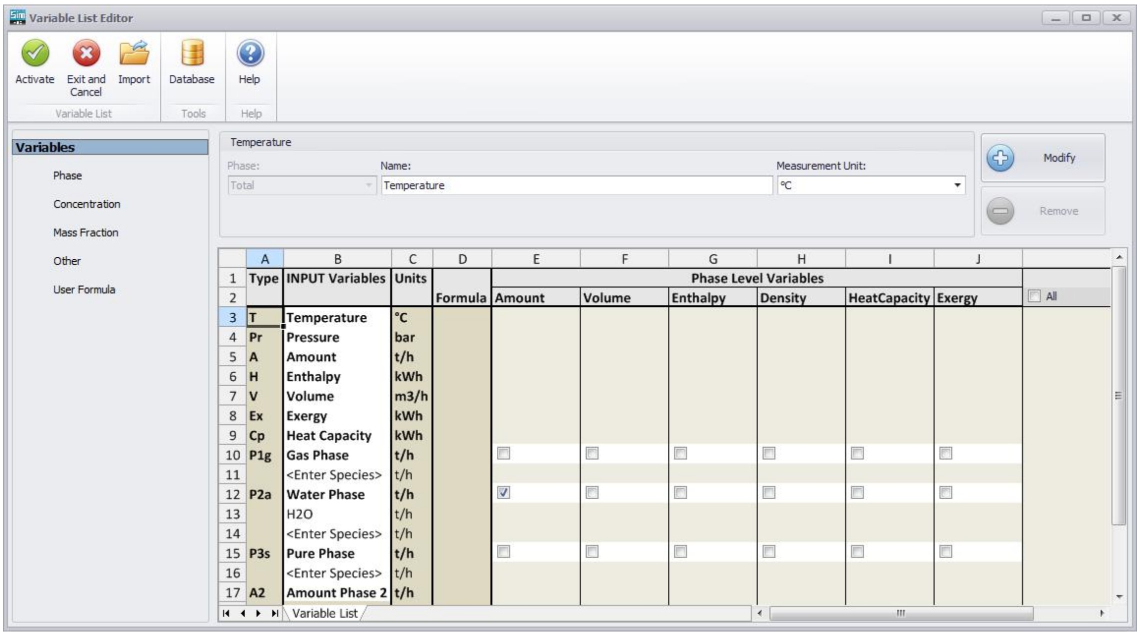


Fig. 3. Variable list of the Cooler unit.

44.2.3. Add Reaction Equations to the Unit (Chapter 43 section 43.3.)

The following leaching reaction equations:

$FeS + H(+a) + O_2(g) = Fe(+2a) + S + H_2O$ (90 % efficiency)

$H_2SO_4 = H(+a) + SO_4(-2a)$ (100 % efficiency)

can be added with the Chemical Reactions Wizard. In the **Leaching unit**, open the Excel editor "Chemical Reactions Wizard". You have to write the Progress %, Reactants, Products, and press the Balance button, which checks the coefficients for the reactions, see **Fig. 4**.

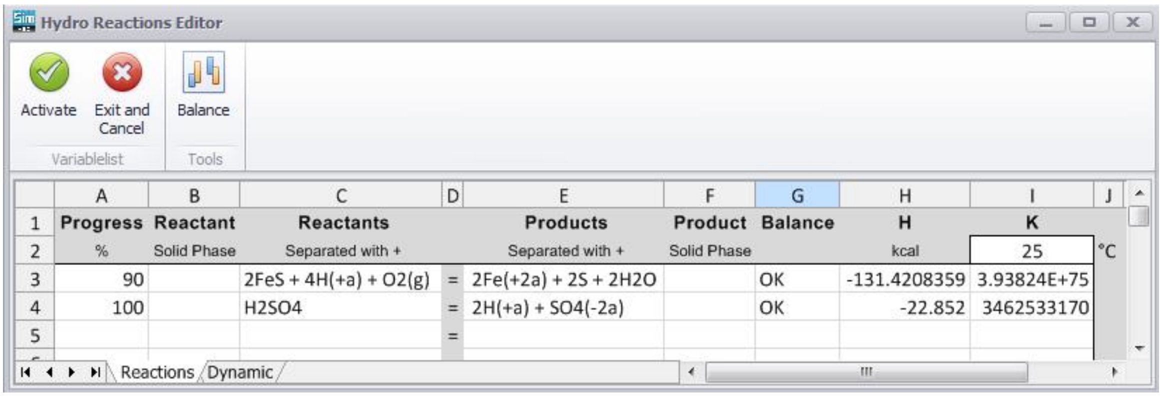


Fig. 4. Reactions sheet in Chemical Reactions Wizard.

44.2.4. Specify Distributions

Remember to complete the **Dist** sheets of the units. In the Leaching unit, 100% of the gas phase goes to the Offgas stream and 100% of the liquid and solid phase goes to the Solution stream. Fill in the percentages for both streams, see **Fig. 5**. In the **Cooler unit** there is just one output stream so fill in 100 % to each phase.

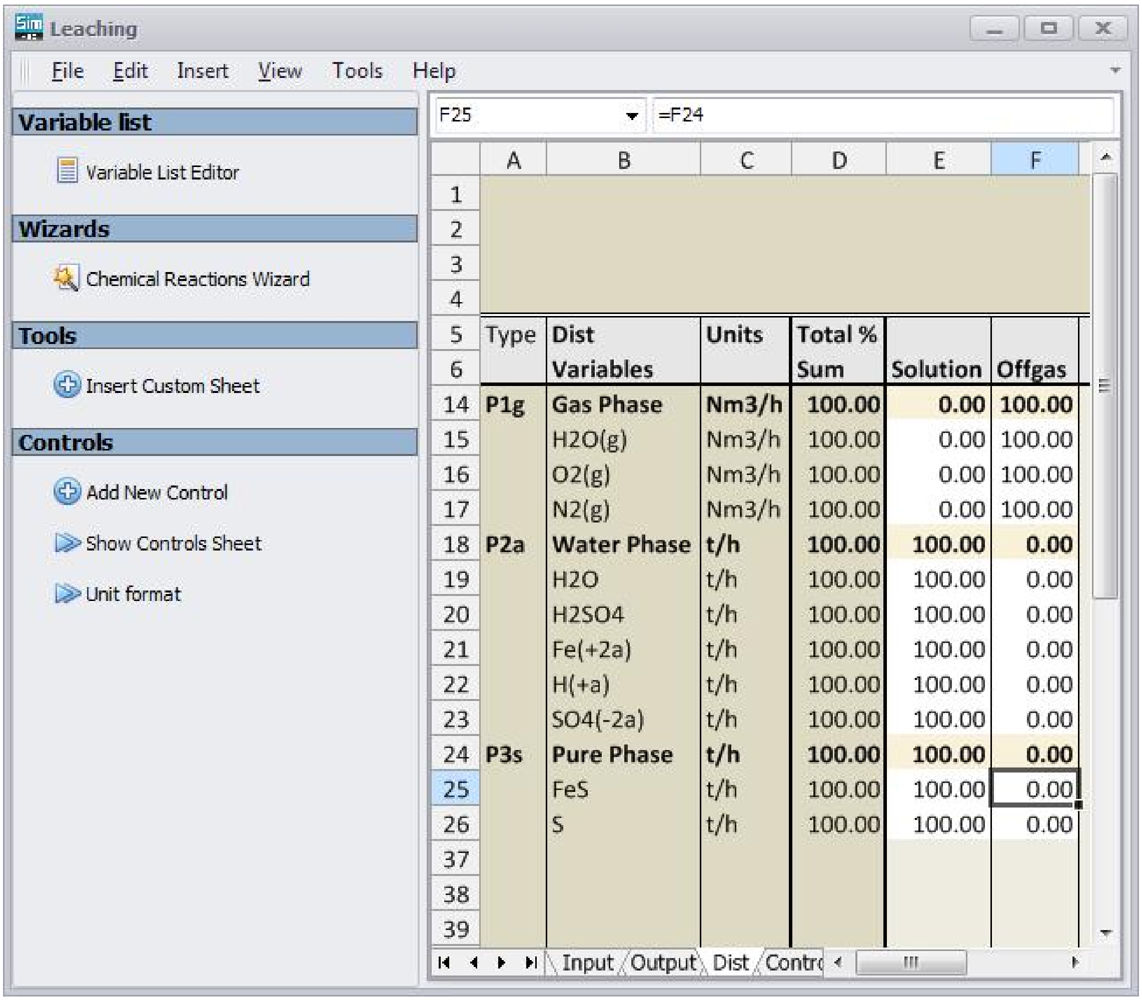


Fig. 5. Dist. sheet of the Leaching unit.

44.2.5. Setting Controls for the Process, Chapter 43 (section 43.5.)

Controls can be added, removed and seen using quick links on the left column, see **Fig. 6**.

In the first control sheet, the H_2SO_4 concentration after leaching is set at 1 g/l of solution by calculating the input amount of H_2SO_4, see **Fig. 6** and **Table 1**.

In the second control sheet, the cooling requirements (heat balance) of the highly exothermic leaching process are set to 0 by calculating the cooling water amount. NB! Insert an extra sheet in the Cooler unit, see **Fig. 7** to **Fig. 10** and **Table 2**.

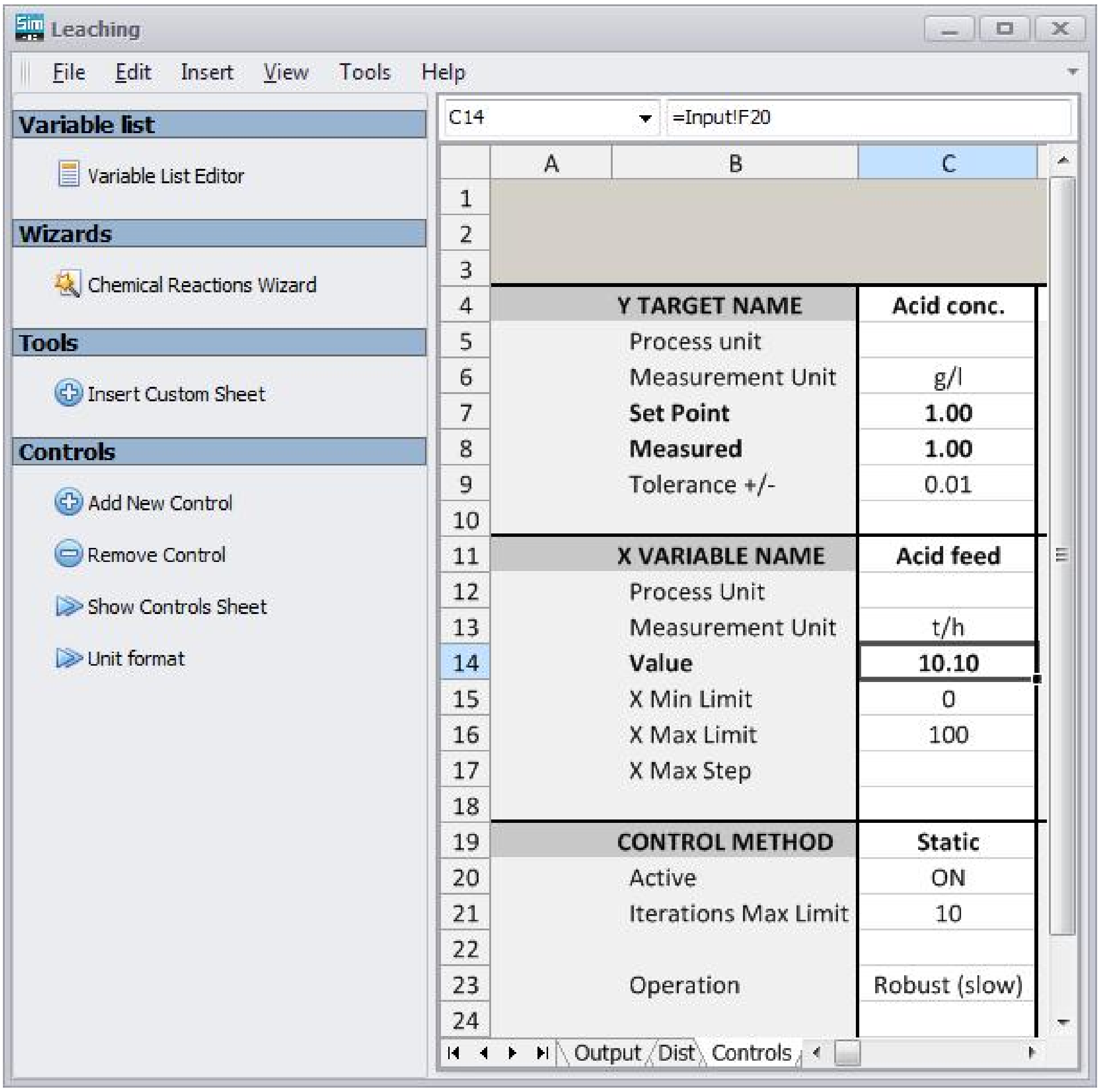


Fig. 6. Controls sheet of the Leaching unit.

Table 1. Data for controlling the H_2SO_4 concentration after leaching.

Row name (Cell)	Filled value or formula	Notes
Set point (C7)	1	Desired H_2SO_4 concentration, g/l
Measured (C8)	=Output!E36	Measured H_2SO_4 concentration, g/l
Tolerance +/- (C9)	0.01	Tolerance for concentration
Value (C14)	=Input!F20	H_2SO_4 input to the process, t/h
X Min Limit (C15)	0	Minimum amount for H_2SO_4 input
X Max Limit (C16)	100	Maximum amount for H_2SO_4 input

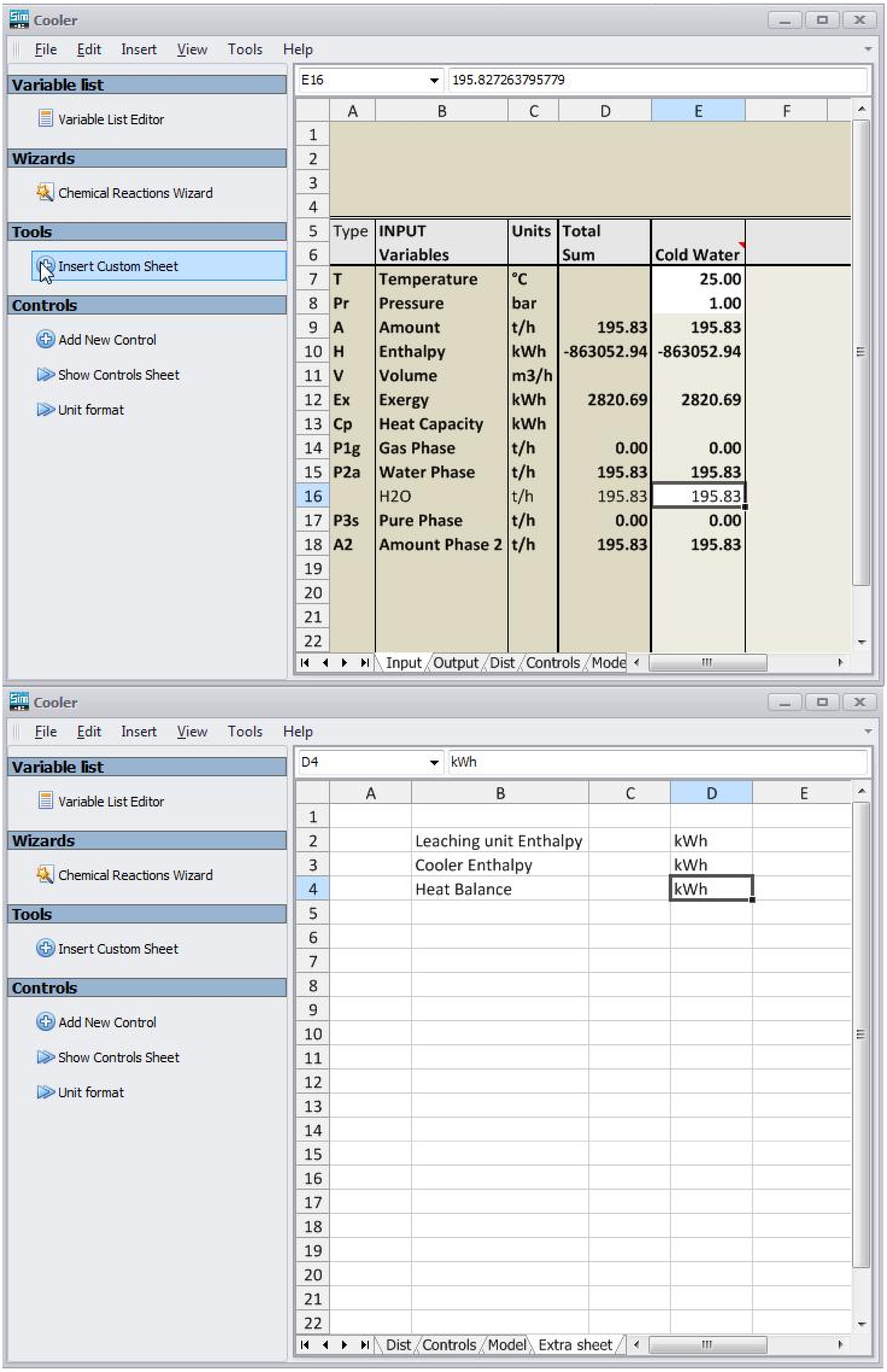


Fig. 7. Insert Custom Sheet and text added to this new sheet (renamed to Extra sheet).

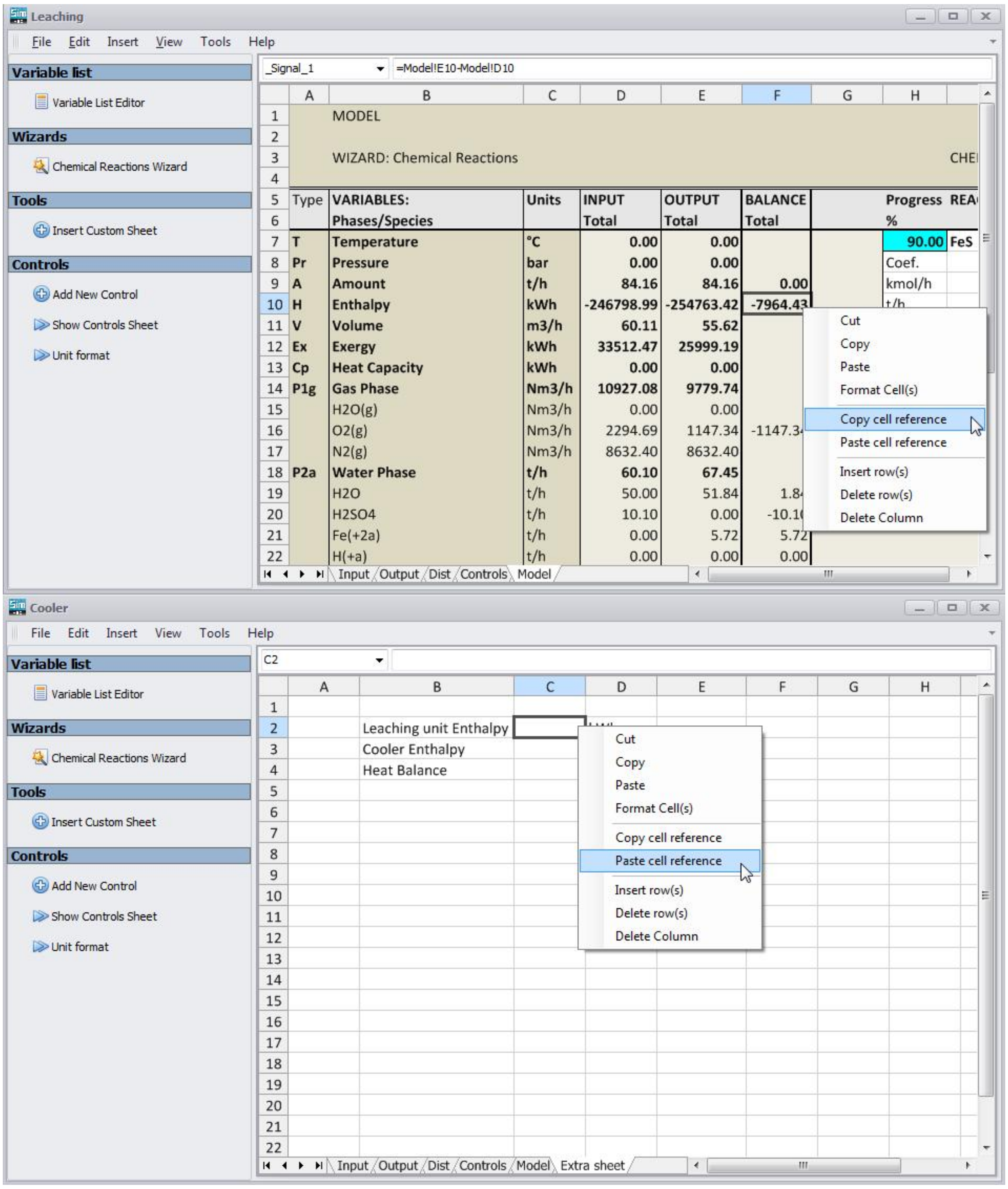


Fig. 8. Copy cell reference from the Leaching unit and paste cell reference to the extra sheet.

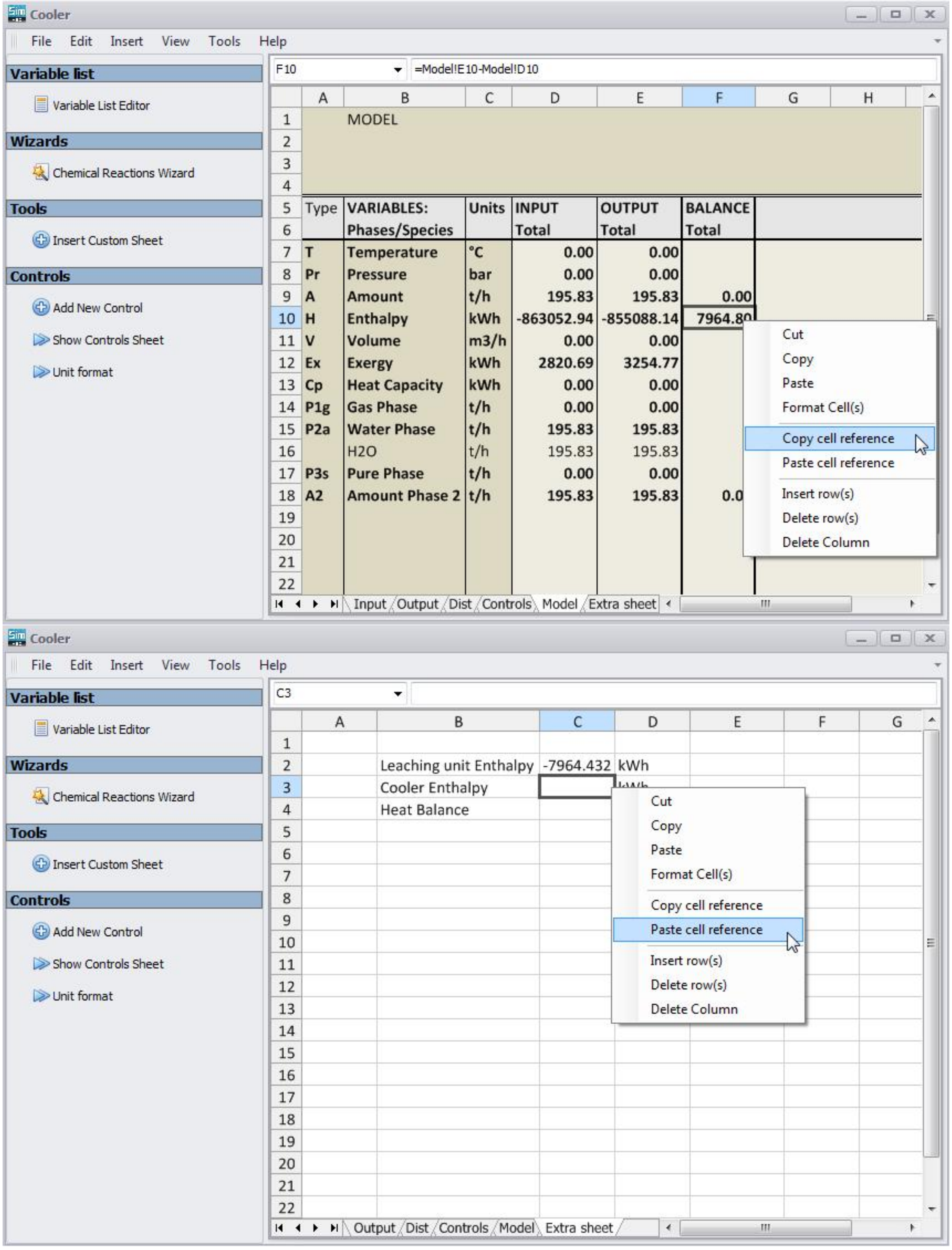


Fig. 9. Copy cell reference from the Cooler unit and paste cell reference to the extra sheet.

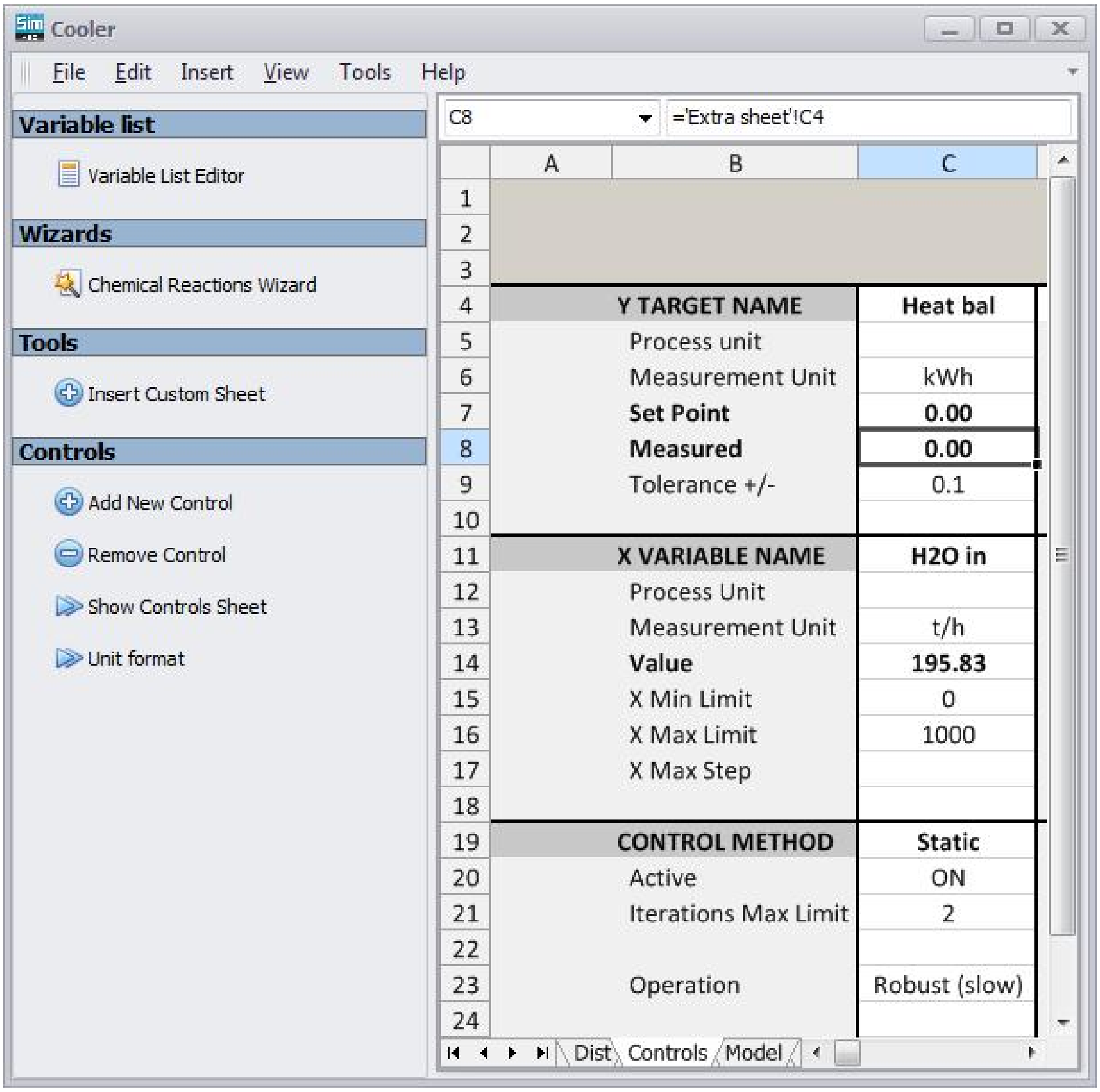


Fig. 10. Controls sheet of the Cooler unit.

Table 2. Data for controlling the Heat balance. Measured value is calculated in an additional sheet.

Row name (Cell)	Filled value or formula	Notes
Set point (C7)	0	Desired Heat balance, kWh
Measured (C8)	=Extra sheet!C4	Measured Heat balance, kWh
Tolerance +/- (C9)	0.1	Tolerance for Heat balance
Value (C14)	=Input!E16	H_2O input to the process, t/h
X Min Limit (C15)	0	Minimum amount for H_2O input
X Max Limit (C16)	1000	Maximum amount for H_2O input

44.2.6. Setting Feed Streams to the Process

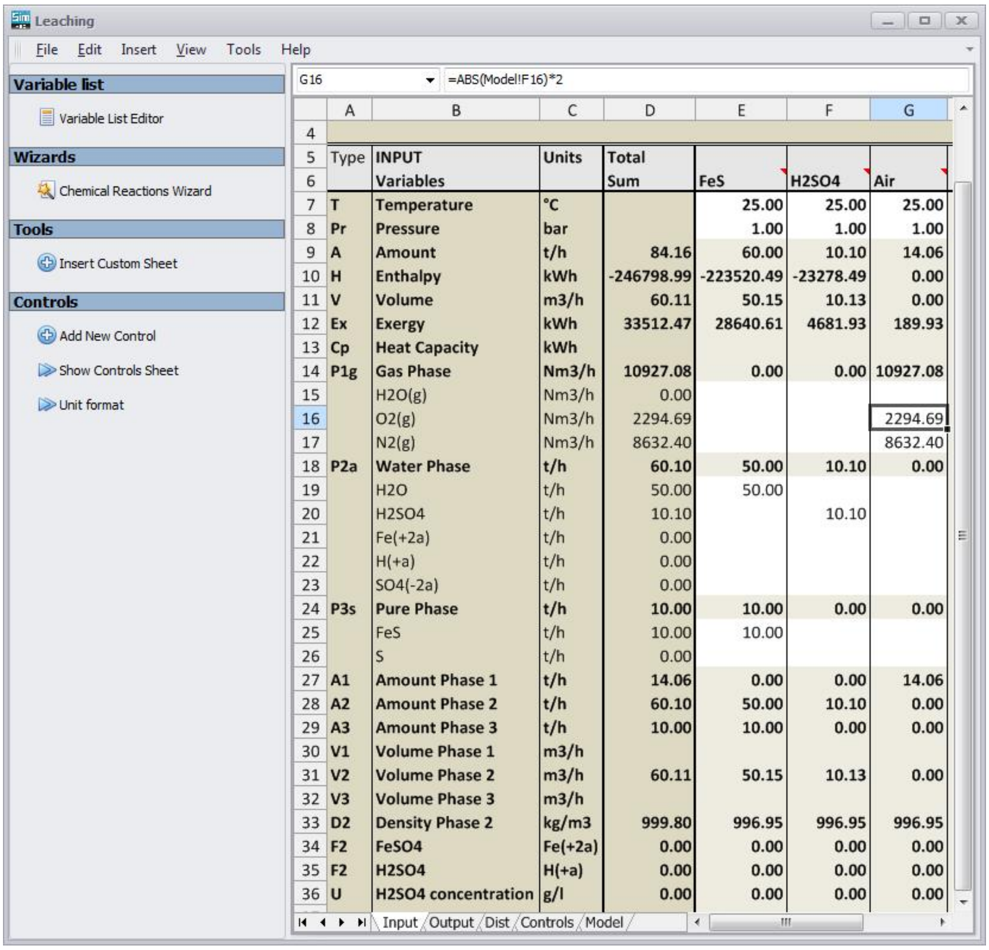
All the **feed streams** to the process should be set. If the feed to the process is not set, the stream will be ignored.

Input sheets of both Leaching and Cooler units:

- FeS stream H_2O is 50 t/h and FeS is 10 t/h in the FeS stream.
- H_2SO_4 stream sulfuric acid feed - an initial guess of 1 t/h can be given. Real value (10.1 t/h) is calculated using the control, see **Table 1**.
- Air stream consists of 21 vol.% of O_2(g) and 79 vol.% of N_2(g). Oxygen efficiency is 50 %, which means that 2 times the stoichiometric amount is needed. The formulas made for oxygen and nitrogen are =ABS(Model!F16)*2 and =G16/21*79, respectively.
- Cold water stream feed - an initial guess of 10 t/h can be given. Real value (195.8 t/h) is calculated using the control, see **Table 2**.

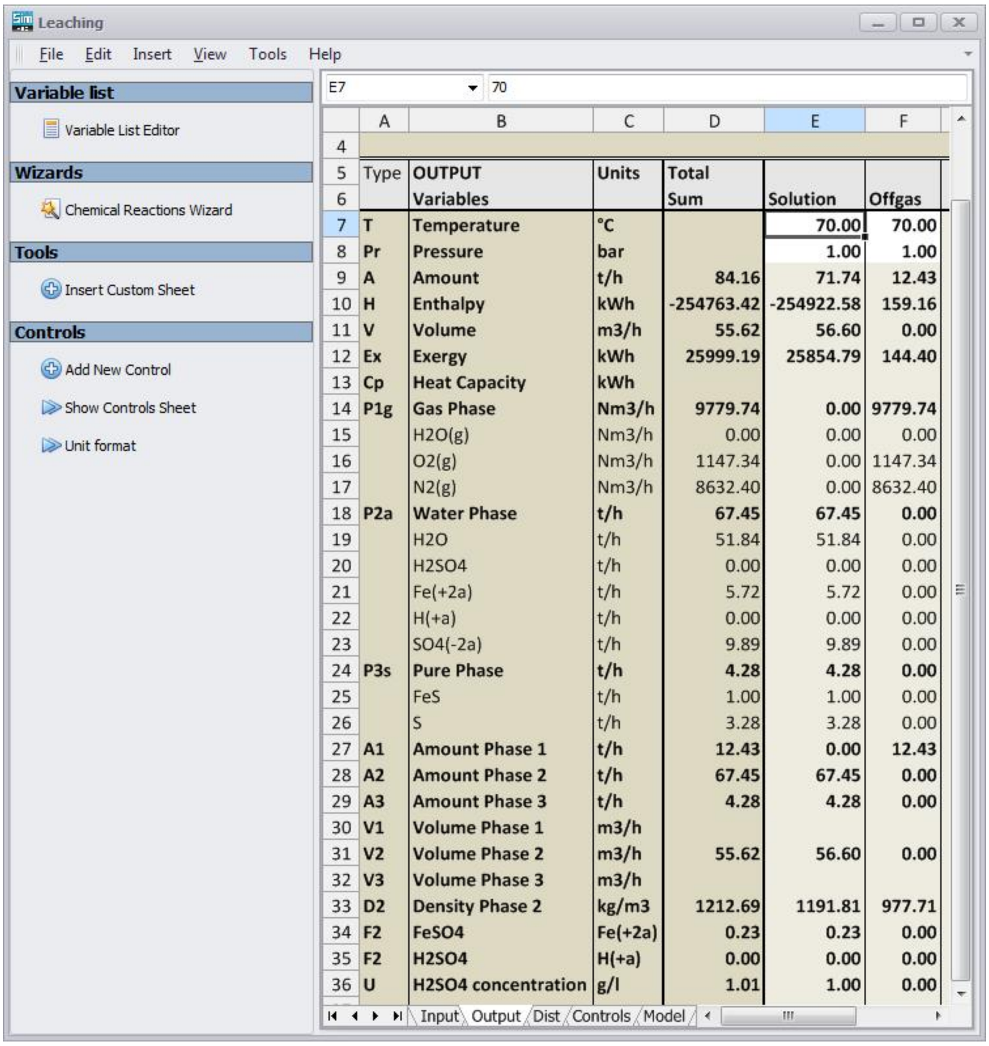
Output sheets of both Leaching and Cooler units:

- Temperature of solution and offgas streams should be set to 70 °C, see **Fig. 12**.
- Temperature of hot water stream should be set to 60 °C.



	A	B	C	D	E	F	G
4							
5	Type	INPUT	Units	Total			
6		Variables		Sum	FeS	H2SO4	Air
7	T	Temperature	°C		25.00	25.00	25.00
8	Pr	Pressure	bar		1.00	1.00	1.00
9	A	Amount	t/h	84.16	60.00	10.10	14.06
10	H	Enthalpy	kWh	-246798.99	-223520.49	-23278.49	0.00
11	V	Volume	m3/h	60.11	50.15	10.13	0.00
12	Ex	Exergy	kWh	33512.47	28640.61	4681.93	189.93
13	Cp	Heat Capacity	kWh				
14	P1g	Gas Phase	Nm3/h	10927.08	0.00	0.00	10927.08
15		H2O(g)	Nm3/h	0.00			
16		O2(g)	Nm3/h	2294.69			2294.69
17		N2(g)	Nm3/h	8632.40			8632.40
18	P2a	Water Phase	t/h	60.10	50.00	10.10	0.00
19		H2O	t/h	50.00	50.00		
20		H2SO4	t/h	10.10		10.10	
21		Fe(+2a)	t/h	0.00			
22		H(+a)	t/h	0.00			
23		SO4(-2a)	t/h	0.00			
24	P3s	Pure Phase	t/h	10.00	10.00	0.00	0.00
25		FeS	t/h	10.00	10.00		
26		S	t/h	0.00			
27	A1	Amount Phase 1	t/h	14.06	0.00	0.00	14.06
28	A2	Amount Phase 2	t/h	60.10	50.00	10.10	0.00
29	A3	Amount Phase 3	t/h	10.00	10.00	0.00	0.00
30	V1	Volume Phase 1	m3/h				
31	V2	Volume Phase 2	m3/h	60.11	50.15	10.13	0.00
32	V3	Volume Phase 3	m3/h				
33	D2	Density Phase 2	kg/m3	999.80	996.95	996.95	996.95
34	F2	FeSO4	Fe(+2a)	0.00	0.00	0.00	0.00
35	F2	H2SO4	H(+a)	0.00	0.00	0.00	0.00
36	U	H2SO4 concentration	g/l	0.00	0.00	0.00	0.00

Fig. 11. Feed stream amounts of the Leaching unit.



	A	B	C	D	E	F
4						
5	Type	OUTPUT	Units	Total		
6		Variables		Sum	Solution	Offgas
7	T	Temperature	°C		70.00	70.00
8	Pr	Pressure	bar		1.00	1.00
9	A	Amount	t/h	84.16	71.74	12.43
10	H	Enthalpy	kWh	-254763.42	-254922.58	159.16
11	V	Volume	m3/h	55.62	56.60	0.00
12	Ex	Exergy	kWh	25999.19	25854.79	144.40
13	Cp	Heat Capacity	kWh			
14	P1g	Gas Phase	Nm3/h	9779.74	0.00	9779.74
15		H2O(g)	Nm3/h	0.00	0.00	0.00
16		O2(g)	Nm3/h	1147.34	0.00	1147.34
17		N2(g)	Nm3/h	8632.40	0.00	8632.40
18	P2a	Water Phase	t/h	67.45	67.45	0.00
19		H2O	t/h	51.84	51.84	0.00
20		H2SO4	t/h	0.00	0.00	0.00
21		Fe(+2a)	t/h	5.72	5.72	0.00
22		H(+a)	t/h	0.00	0.00	0.00
23		SO4(-2a)	t/h	9.89	9.89	0.00
24	P3s	Pure Phase	t/h	4.28	4.28	0.00
25		FeS	t/h	1.00	1.00	0.00
26		S	t/h	3.28	3.28	0.00
27	A1	Amount Phase 1	t/h	12.43	0.00	12.43
28	A2	Amount Phase 2	t/h	67.45	67.45	0.00
29	A3	Amount Phase 3	t/h	4.28	4.28	0.00
30	V1	Volume Phase 1	m3/h			
31	V2	Volume Phase 2	m3/h	55.62	56.60	0.00
32	V3	Volume Phase 3	m3/h			
33	D2	Density Phase 2	kg/m3	1212.69	1191.81	977.71
34	F2	FeSO4	Fe(+2a)	0.23	0.23	0.00
35	F2	H2SO4	H(+a)	0.00	0.00	0.00
36	U	H2SO4 concentration	g/l	1.01	1.00	0.00

Fig. 12. Output stream temperatures of both Solution and Offgas streams are put at 70 °C.

44.2.7. Saving the Process, Chapter 40 (sections 40.2. and 40.3.1.)

Processes should always be saved in their own folder. Changing the process name is not enough since every unit is an Excel file that is saved in the same folder as the flowsheet. The name of these files is the same as the name of the units. Therefore you also have to save different scenarios in different folders.

44.2.8. Running the Simulation and Checking the Results, sections 40.3.1 and 40.3.2

When you have finished the model you can run the simulation. First you have to set the number of rounds you wish to calculate the process and then press the Simulate button to start the simulation. You should check if the values change during different runs to find out if the process is in balance. The value of the selected variable is presented in the value labels, see **Fig. 13**. User can add Stream Tables and Header (Chapter 40 sections 40.1.4 and 40.3.1) to visualize the calculation results, see **Fig. 14** and **Fig. 15**.

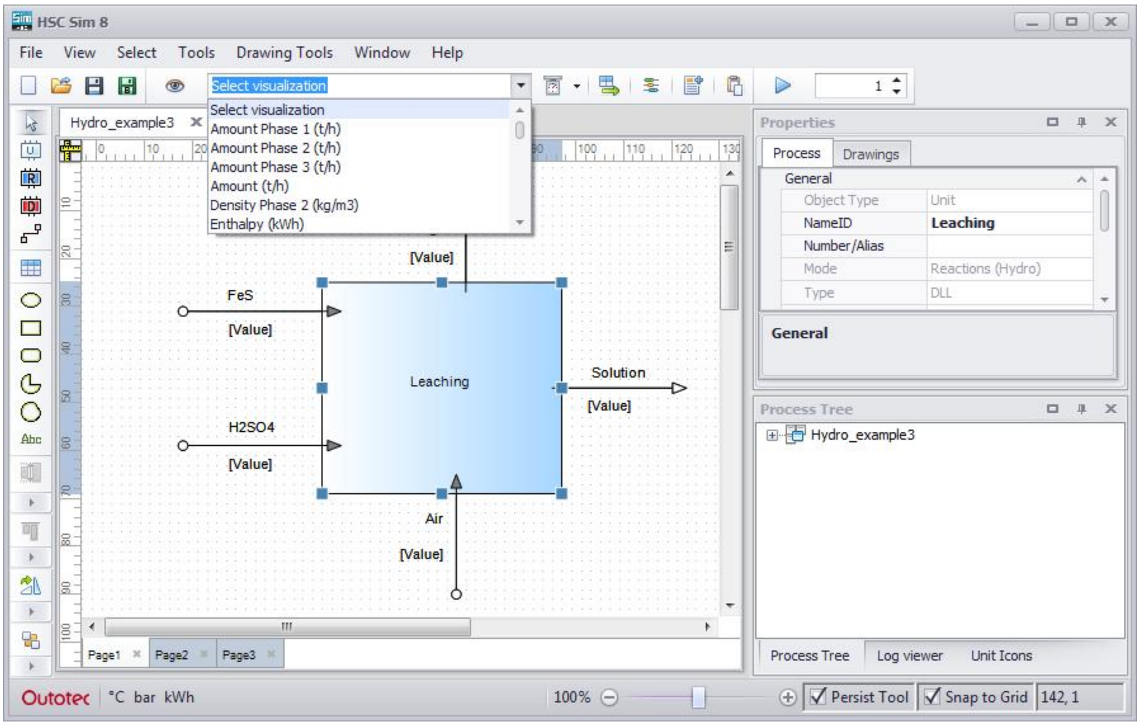


Fig. 13. Selecting visualization from the list.

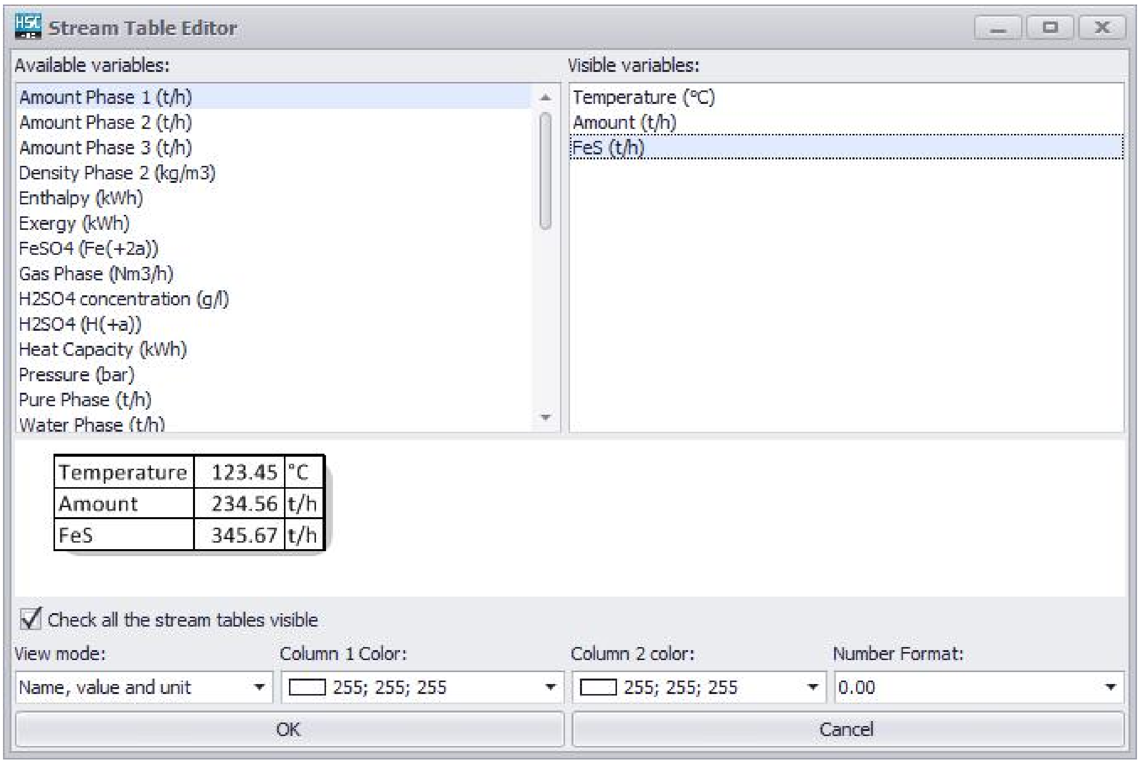


Fig. 14. Stream Table Editor to modify Stream Tables.

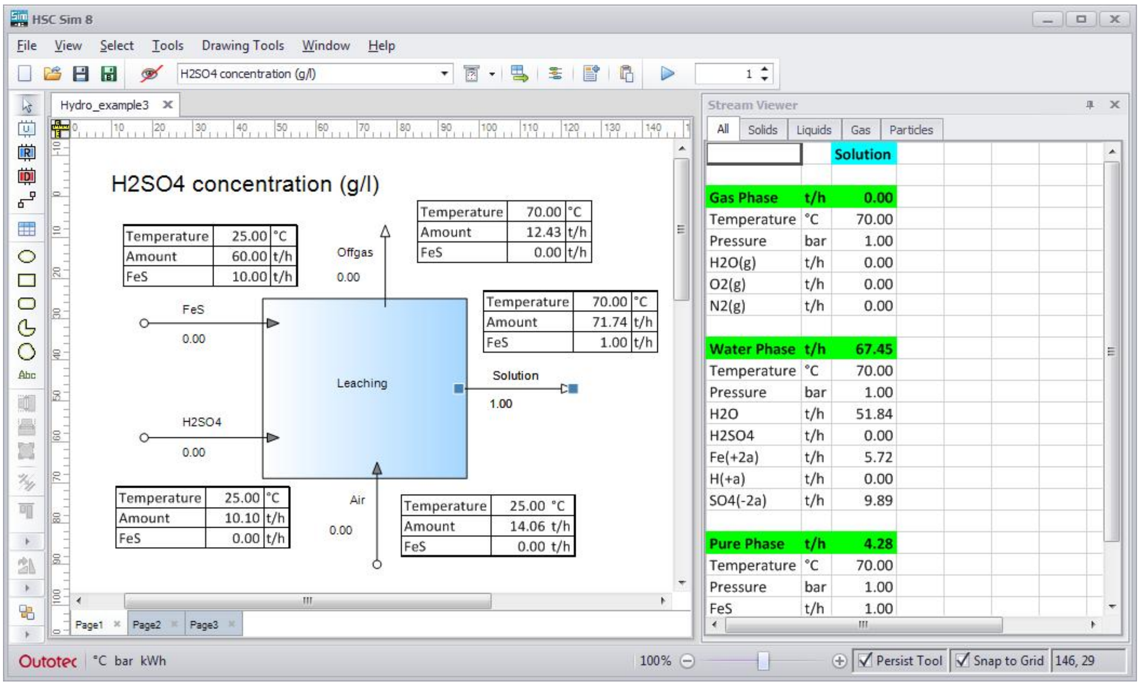
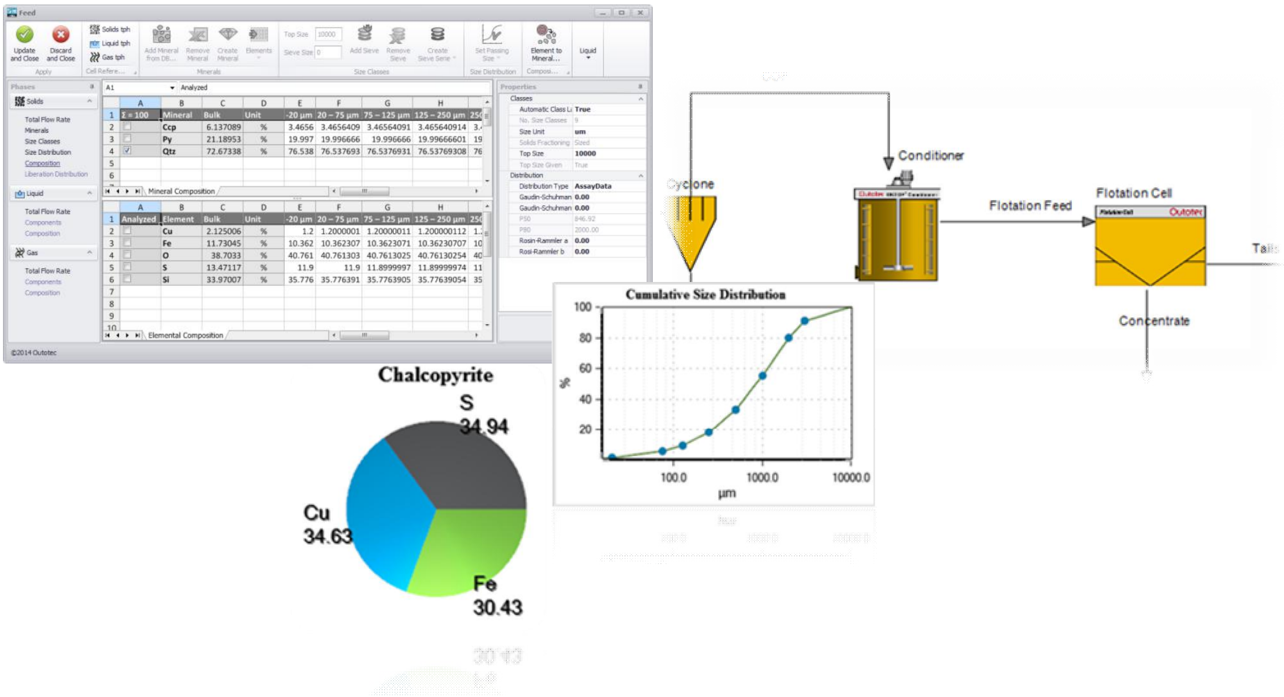


Fig. 15. Stream Tables and Stream Viewer to visualize calculation results.

45. Sim Minerals Processing



TOC:

45.1. Introduction

45.1.1. Particle-based modeling

HSC Sim has a special set-up and approach for processes where minerals are treated. This approach should be used for processes such as crushing, grinding, flotation, gravity separation and screening. Mineral-based models treat particles that have at least the following properties:

- size (diameter)
- mineral composition in wt.%

In addition, they may have additional parameters like composition by volume%, mineral composition by surface area%, whiteness, hardness, etc. Each mineral has a certain chemical composition and specific gravity on the basis of which HSC will calculate these properties for each particle and also for each stream. **Fig. 1** illustrates the solids phase set up as a particulate material - the approach HSC Sim minerals processing models are based on.

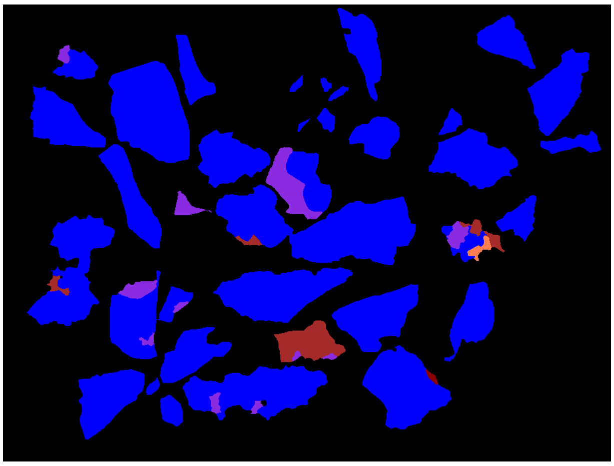


Fig. 1. Particles of different sizes, consisting of one or more minerals. A colored SEM (Scanning Electron Microscope) graph (Outotec Research, Pori, Finland).

HSC Sim supports a versatile set-up of the particle-based feed streams, according to the desired modeling complexity. Each mineral can be a fully liberated material that can be further be divided into several size classes with particles in them. With a more elaborated feed set-up, the degree of liberation and association between different minerals in each size class can be defined. **Fig. 2** gives examples of different particle set-ups: liberated (100% one mineral), binary (two minerals), ternary (three minerals), and complex (four or more minerals); all of these are possible in HSC Sim.

The feed composition and mineralogy are defined with the HSC Sim Stream Setup tool complemented by HSC Geo's extensive mineral database, mineralogical calculation tools, and MLA (Mineral Liberation Analysis) data file importing and handling possibilities.

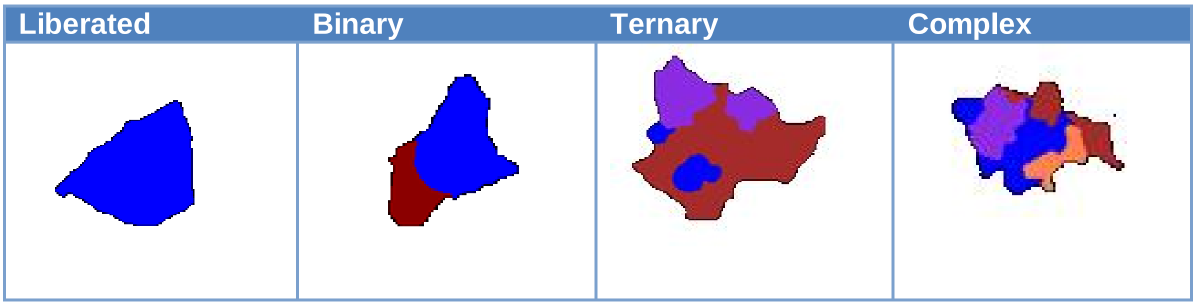


Fig. 2. Different complexities of minerals according to their liberation.

HSC Sim assigns several properties to each particle. A stream consists of a certain ton per hour amount including that particle type. All the stream properties, such as the element wt% in it, solid specific gravity, or total solids tons per hour, for example, are always calculated based on the particle composition of the stream. The particle properties and most common stream properties are listed below. These stream properties are also at the same time the initial data for setting up a feed stream for which the particles are automatically generated.

1. <u>Particle properties</u>

Each particle has its own specific properties that are set when they are created, e.g. in the feed Stream Setup. They consist of:

- A list of minerals, their composition% in a particle and properties including:
  - ✓ Name
  - ✓ Code (name shortening)
  - ✓ Chemical formula
  - ✓ Specific gravity
  - ✓ Chemical composition
  - ✓ *Optional: Database reference*
  - ✓ *Optional: additional properties (user-defined)*
- Size class information including:
  - ✓ Lower and upper boundary of each class and geometric average
  - ✓ Name label of the size class
  - ✓ Optional: number of particles in a class, in case of MLA file imported particles
- *Optional: particle floatability parameters for flotation kinetics based separation*
- *Optional: particle type, indicating its mineral association group, typically with MLA file imported particles.*

2. <u>Stream properties (feed)</u>

Streams consist of numerous properties and calculated values derived from their particle composition. The feed stream particles are generated by HSC Sim based on the following data:

- Total solids input of the stream (t/h)
- Weight percentage of each size class (totaling 100%)
- Weight percentage of each mineral in each size class (totaling 100%) and in bulk (calculated)
- Chemical composition of fractions and bulk (calculated)
- *Optional: mineral liberation and association data for each size class. Only if non-liberated particles are to be set up and used in modeling.*

Particle handling in process units:

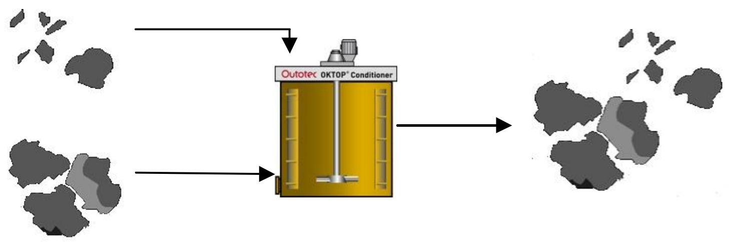
When a stream is directed to a certain unit in a flowsheet, the particular unit operation of that unit can treat the particles as follows:

1. Mix the particles of all the incoming streams and direct the mixture to one or more outputs.
2. Break down the particles. This is the only unit operation where (some of) the incoming particles are destroyed and do not exist in the output. Instead, new particles are generated so that the total flow rate and mineral balance are held over the unit.
3. Particles can be separated according to several properties; typically: size, specific gravity, mineral composition (resulting in the overall flotation kinetics for that particle, for example), etc…

The above main particle stream phenomena and examples of the unit operations for these are shown in **Fig. 3**.

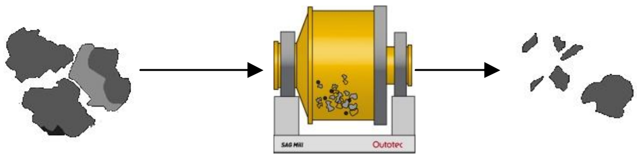
Mixing

- **Pump sump**
- **Feed box**
- **Mixing tank**
- **…**



Breaking Down

- **Crushing**
- **Grinding**
- **…**



***Separation*, by**

- **Size (e.g. screening, hydrocyclones)**
- **Specific Gravity (e.g. Knelson concentrator, hydrocyclones)**
- **Mineral Composition (e.g. flotation)**
- **Shape, Color, etc…**

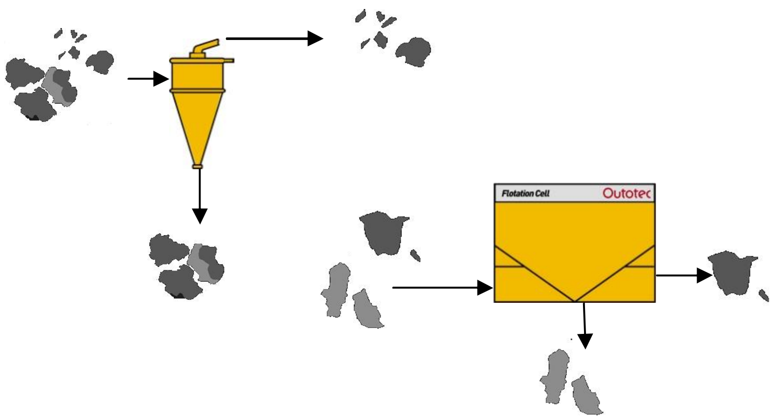


Fig. 3. Examples of unit operations based on the stream particles.

45.1.2. Levels of modeling detail

Before starting to build up HSC Sim minerals processing models it is worth considering how much detail is required, what background data are available, and what type of unit models are available with what level of detail. **Fig. 4** illustrates how the feed material can be defined and thus how the unit models should be capable of handling stream compositions.

In addition to increasing the level of detail, the number of particles transferred between the units increases. With large simulation models this might have impact on the simulation calculation speed (especially in the case of dynamic simulation). Also, quite often increasing the modeling details means increasing the time needed to build up and parameterize the simulation model. **Fig. 5** lists some of the minerals processing application areas where different details of modeling are typically applied.

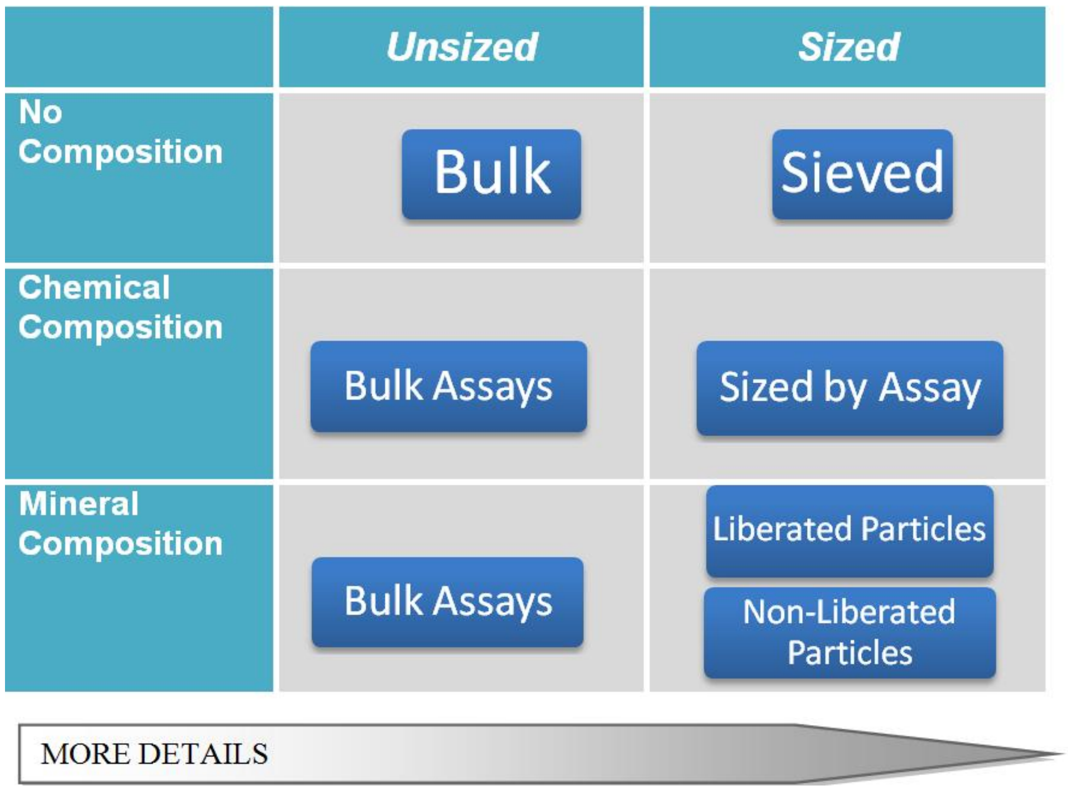


Fig. 4. Levels of modeling detail – required background data.

	Unsized	*Sized*
No Composition	▪ Simple Material t/h Balance	▪ Crushing ▪ Grinding ▪ Screening ▪ Cyclones ▪ Etc...
Mineral / Chemical Composition	▪ Bulk Material: ▪ Flotation ▪ Physical Separation ▪ Etc...	▪ Sized Particles: ▪ Flotation ▪ Physical Separation ▪ Comminution ▪ Etc... ▪ *MLA Based Particles Modeling*

Fig. 5. Levels of modeling detail – examples of modeling application areas.

45.1.3. Minerals processing flowsheet structure in HSC Sim

The HSC Sim process flowsheet consists of Units and Streams (**Fig. 6**). When the modeling is based on particles, a ***Stream*** consists of ***Solids*** and ***Liquid*** and ***Gas*** phases, although the gas phase is rarely set for a mineral slurry feed stream. The liquid may have soluble components, but in minerals processing, these species are often ignored, i.e. the liquid (water) only has density as a parameter. Solids consist of particles which are composed of minerals. Minerals have properties such as chemical composition. In HSC Sim all the properties of solids are calculated from particle flow rates, particle compositions, and mineral properties. For example, copper does not behave independently in the process but is always bound to a mineral or minerals that occur in particles, which vary in size and composition.

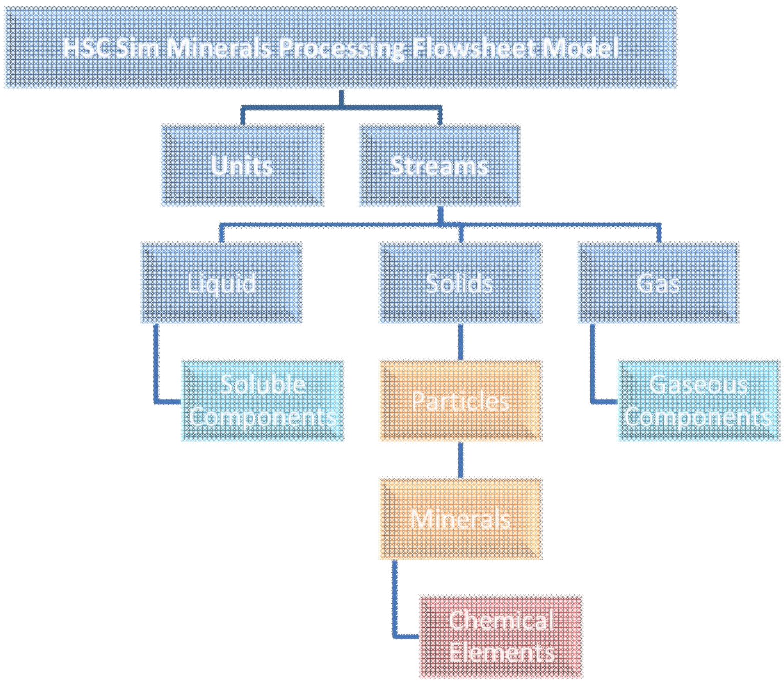


Fig. 6. Structure of HSC Sim flowsheets for minerals processing.

45.1.4. HSC Sim file structure

HSC Sim flowsheet models must always be *saved in a separate folder*, each of them. This is because the same file names may exist in the flowsheets, and they must not be mixed between flowsheets. The folder name can differ from the flowsheet name; they are not related to each other. The process flowsheet model is in a ***Sim8*** file, and can be opened in HSC Sim 8 by double-clicking it. **Table 1** summarizes the simulation model files located in the model folder.

NB: A flowsheet model can be copied or sent elsewhere just by sending (zipping) the whole simulation model folder.

Table 1. HSC Sim files in minerals processing flowsheet models.

Model Component	Corresponding Files	What They Are
Flowsheet	ProcessName.**Sim8** ProcessName.**Sim8bin**	▪ Flowsheet layout description ▪ Unit icons, data, etc. related to the flowsheet
Unit	Unit_1.**xlsx** Unit_2.**xlsx** Unit_N.**xlsx**	▪ Each unit has a separate file to store its parameters, state and settings
Feed Stream	Feed_1.**HSCStream** Feed_2.**HSCStream** Feed_N.**HSCStream**	▪ Each feed stream has a separate file to describe the (particle) feed composition

45.1.1 Before starting to create a simulation model

Before starting to build a process for simulation, you should collect all the relevant data of the process. According to the data and your aims, you should:

1. Decide the level of detail you want to have in the drawing and simulation.

   - Is it necessary to draw all the existing units (e.g. pump sumps), or could the circuit be simplified without losing any essential information?
   - It is a good idea to draw a draft of the flowsheet on a piece of paper. That will help you to position the units correctly.

2. Decide the level in terms of particles. The possible levels from the lowest (least information) to the highest are:

   a. **Sized model without composition.** Typically grinding circuits are modeled like this. The chemical and mineral composition of the input (e.g. ROM) is identical to the output (e.g. flotation feed), and the main interests are in flow rates and the required energy. (Typically 5-25 particles)

   b. **Unsized mineral model.** Each mineral is treated separately but all the size classes are treated together. Typically a simple flotation model is like this. (Typically 3-8 particles)

   c. **Unsized floatability components model**. Each mineral is divided into 2-3 floatability classes, (i.e. fast floating, slow floating and non-floating) or several (~20) different classes of floatability distribution (e.g. Klimpel model). (Typically 9-150 particles)

   d. **Size-by-mineral model.** Each mineral is treated (Typically 15-

	separately by size. This approach enables the simulation of a full mineral processing circuit including crushing, grinding, classification, and different kind of separation techniques like flotation, gravity separation, magnetic separation, and dewatering.	300 particles)
e.	**True particles model.** This is the highest level of modeling where particles treated in the process have been measured with e.g. MLA and all of them or groups formed from them are treated in the process.	(Typically 200-15 000 particles)

Remember that if you go to a higher-level approach you will need more data and better models.

3. List the minerals present in the circuit. Find their chemical composition and specific gravity. If you do not know, please ask a geologist or mineralogist or look for a mineralogical report.

4. Find the chemical composition or mineral composition of the feed streams. If you have only the chemical composition, do the element to mineral conversion (with HSC Geo, together with the Sim Stream Setup tool).

5. Find the flowsheet of the process or if it is a greenfield process, consider possible alternatives and decide where to start.

6. Find data for unit models and their parameters. To create models you will need some experimental data. These are elemental assays from a laboratory test, pilot test, or survey. If you have data, you can organize the data in HSC using the Mass Balance module to mass balance and reconcile data (see Chapter 51 Mass Balance). Some of the simplest models do not have operational parameters like size, length, gap size, volume, or area, but if you want to use more comprehensive models you should gather this information as well.

After obtaining the background data, the building of a simulation model comprises the following main steps:

I. Draw the flowsheet: place the units there, rename them, draw the streams and rename them
II. Check that all the streams are connected correctly
III. If not yet done, next save the flowsheet to a separate folder. Please take backups every now and then
IV. Define the feed streams: feed rate, select minerals, size classes, size and mineral/elemental composition, liquid and gas phases
V. Select and load the unit models and set the parameters and possible controls for them
VI. Simulate and fine-tune the model. View, visualize and report the results.

These steps are described in more detail in the following sections.

45.2. Drawing a flowsheet

45.2.1. Units and unit icons

The process units can be placed by dragging and dropping them from the Unit Icons panel on the right; the library includes several ready-made process device icons. Alternatively, you can just draw a rectangle unit without a figure, by selecting it from the left-side button bar. The unit figure can also be changed and replaced with your own drawing or photograph if desired. Selecting and drawing the unit on the flowsheet are shown in **Fig. 7**.

NB: Unit figures do not contain calculation models, just the graphics to illustrate them on the flowsheet. The calculation model is selected and loaded separately in a later step.

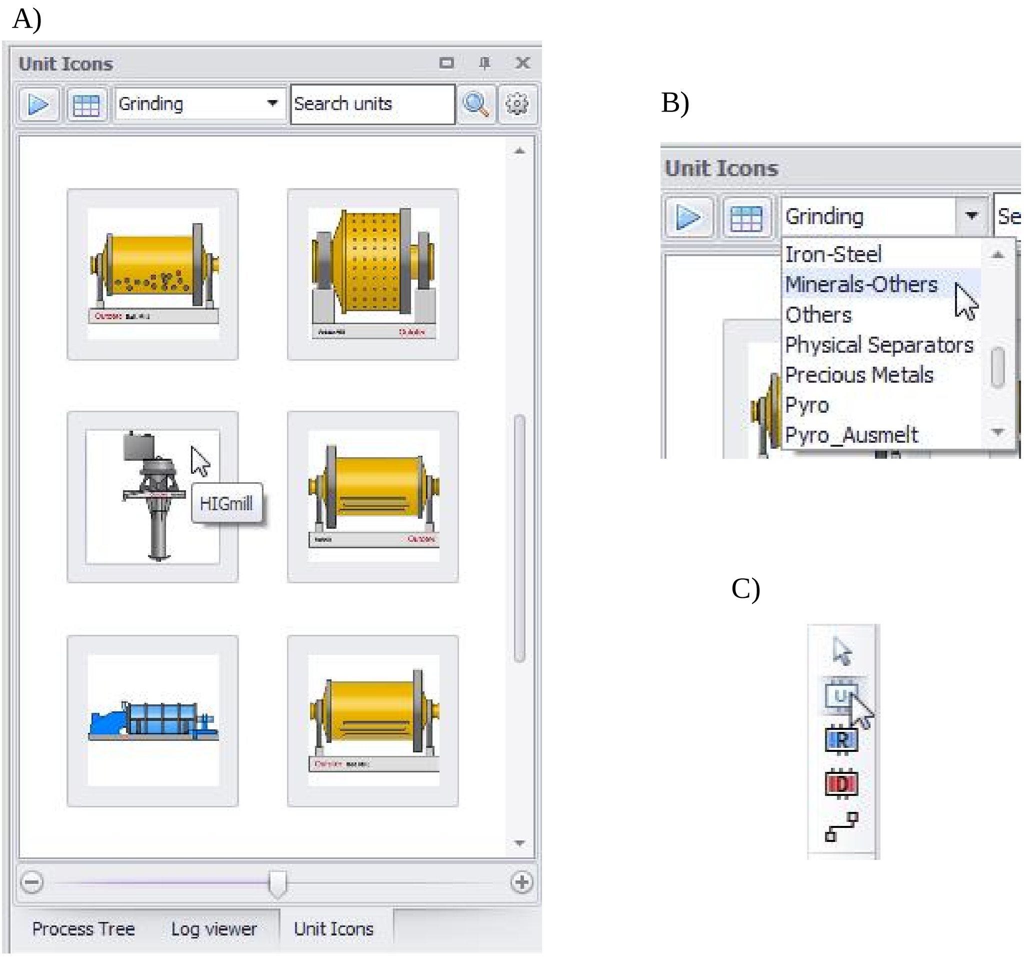


Fig. 7. Unit model icons can be A) dragged and dropped from the HSC Sim library, B) the library folder can be changed from the menu; or C) just a generic unit with a rectangle box icon can be drawn.

45.2.2. Connecting streams

The streams area drawn on the flowsheet by selecting the stream drawing tool from the bar on the left (**Fig. 8**). The streams area is automatically connected to the nearby unit to/from which they are directed. The streams can be redirected and connected elsewhere on the flowsheet; HSC Sim will then ask you to confirm whether the stream source/destination should also be changed (**Fig. 9**). In addition, the source and destination can be set from the stream properties panel on the right (**Fig. 10**).

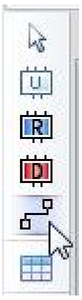


Fig. 8. Drawing the streams.

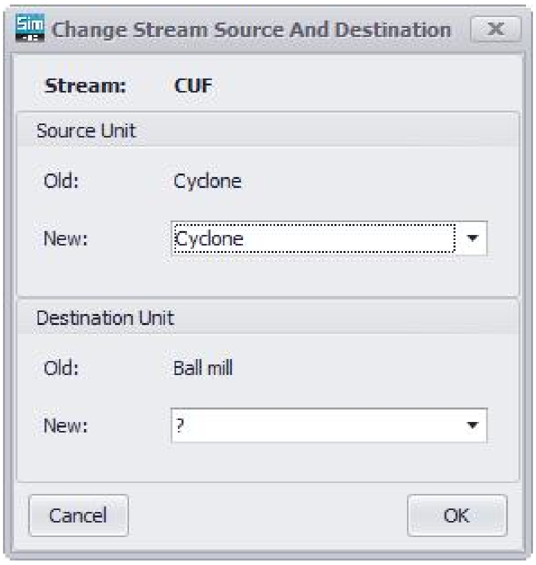


Fig. 9. Setting stream source and destination after redirecting the stream on the flow sheet drawing.

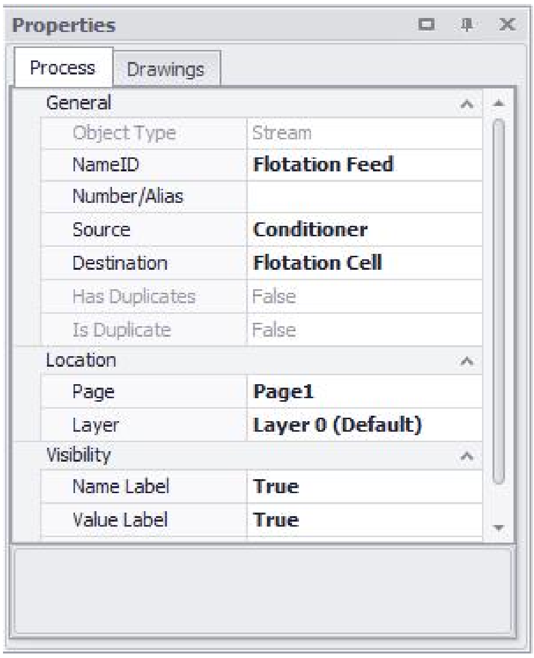


Fig. 10. Stream properties where the Source and Destination can be set.

The streams are renamed by double-clicking the stream name label, or from the stream properties panel. The value labels – showing the simulated values of the selected variable in the visualization mode – are inserted automatically. The stream names and value labels can be modified in terms of font, color, etc. from the properties panel.

45.2.3. Checking the flowsheet

When the flowsheet is ready, you should check that all the stream connections are going to the correct units. The visual notation for the streams is as follows:

- ✓ Starting point = no shape: stream is an output of a unit
- ✓ Starting point = white circle: stream is a feed input to the simulation
- ✓ Ending point = filled arrow: stream goes to an input of a unit
- ✓ Ending point = white arrow: stream is an output of the simulation that does not go to any unit

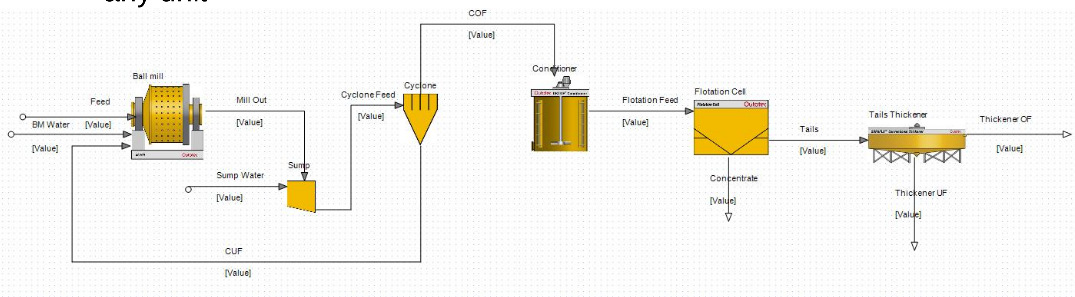


Fig. 11. Example of a flowsheet with units and the streams connecting them.

<u>NB</u>: There is no need to define the stream type as solids/slurry or liquid/water as required in HSC 7. HSC 8 handles all of the streams in the same manner regardless of the stream composition.

When the flowsheet is ready and you have checked it is correct, the feed stream(s) can be defined.

45.3. Stream Setup – Defining the feed composition

Feed Streams for HSC Sim minerals processing models are defined by using the **Stream Setup** tool. To open Stream Setup:

- ✓ Right-click a feed stream and select “Define this stream with Stream Setup”
- ✓ When the stream content is already defined, it can be modified at any time. Open Stream Setup by double-clicking the stream.

The Stream Setup dialog (**Fig. 12**) consists of:

- Upper bar buttons
- Left-side **Phases** navigation tool
- Right-side **Properties** of selected component
- Right-side **Graphs** of selected component
- Middle area for setting up the feed properties

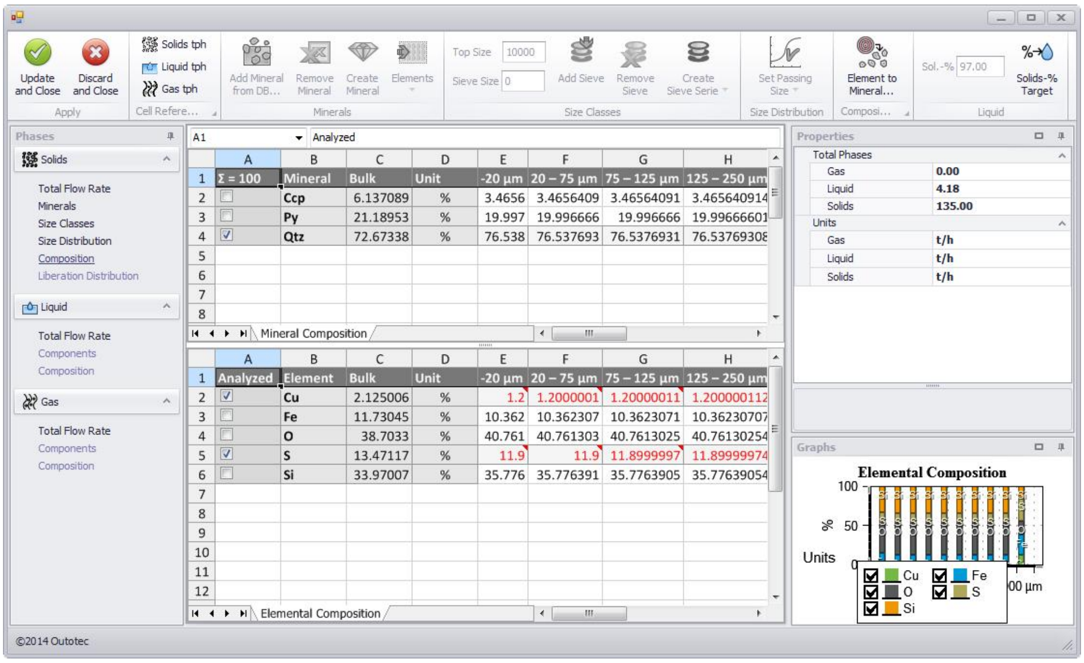


Fig. 12. Stream Setup tool dialog for defining a minerals processing feed stream. The ‘Solids Composition’ view is shown here.

All the required data is entered in the middle part of the dialog, by navigating the steps on the left-side **Phases** navigation panel (**Fig. 13**). The data can be entered in any order, but the easiest way is to follow the links from top to bottom, starting from the Solids Total Flow Rate.

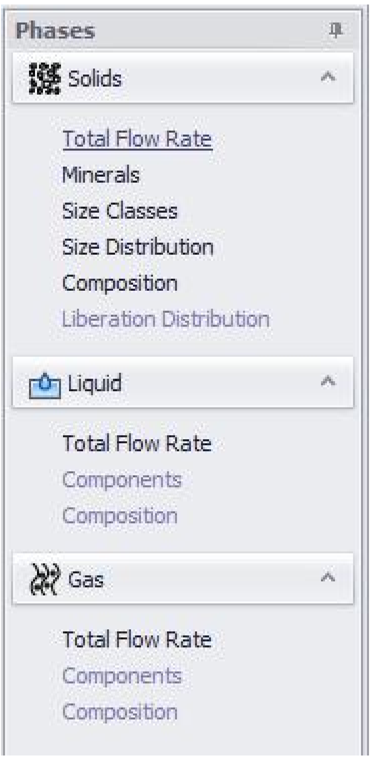


Fig. 13. Phases navigator to set the stream data step by step.

When the desired stream data have been entered, the stream and its particle content are saved and updated to the simulation model by clicking Update and Close on the upper bar (**Fig. 14**). Alternatively, the changes can be cancelled using the Discard and Close button.

The cell references for the total t/h flow rates of the Solids, Liquid and Gas phases can be copied by clicking the respective upper bar buttons. The cell reference can then be pasted and used elsewhere, for example in controls that adjust the flow rates of the feed streams.

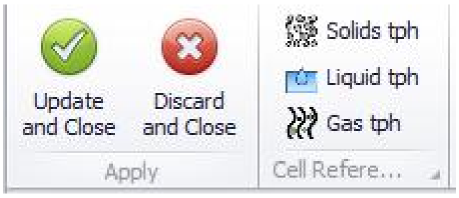


Fig. 14. Buttons to apply changes and to copy cell references for the total phase flow rates.

<u>Good to know:</u>

- ✓ You can always relocate or detach the dialog components as you like
- ✓ Just drag and drop them to undock & dock elsewhere
- ✓ You can leave the dialog components floating on the display and resize them freely
  The figures have tools that appear when you place the cursor over them: you can copy, print, clone, etc.

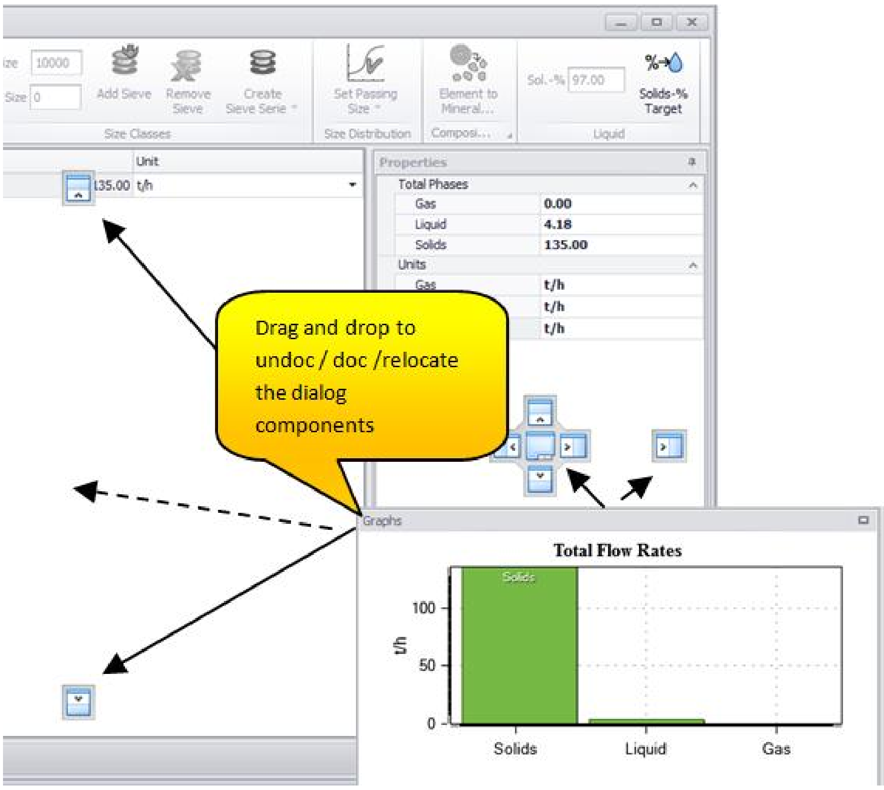


Fig. 15. Relocate and resize the dialog components by undocking and docking them with the left mouse button held down.

45.3.1. Solids feed

Solids feed is based on particles in the HSC Sim minerals processing models (see **Fig. 6**). In the simplest form no size classes (bulk flow) and no minerals are defined (thus the default is bulk 'Ore' mineral). To set up the solids feed composition and mineralogy, the following data need to be defined:

- Total Flow Rate
- Minerals
- Size Classes
- Size Distribution
- Composition of minerals and elements

45.3.1.1. Total solids

The total solids are entered in the Amount field; the unit can be changed from the dropdown menu, and the amount is then automatically recalculated (**Fig. 16**). NB: The unit in this selection does not affect the unit shown in the flowsheet simulation. There the flow rates are shown in t/h.

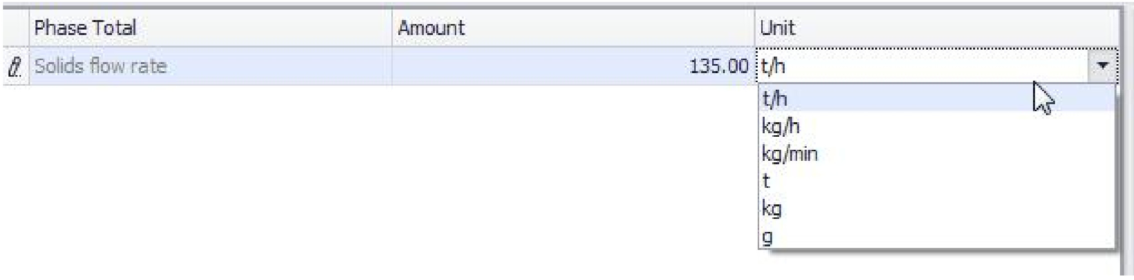


Fig. 16. Setting the total solids flow rate and its measure unit.

In addition, the total phase flows can be entered and the measure units changed in the properties panel on the right (**Fig. 17**).

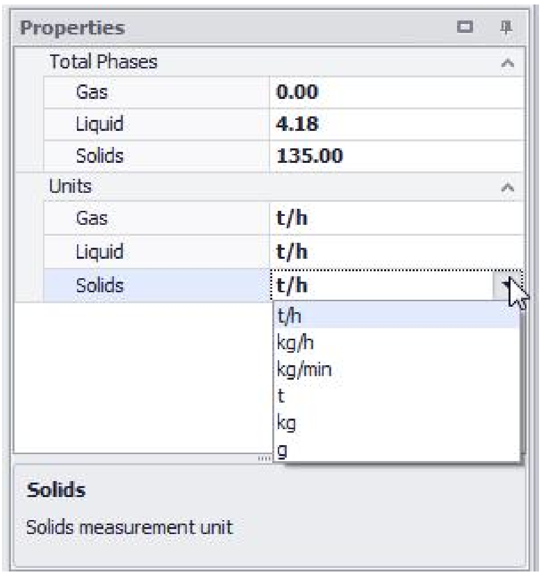


Fig. 17. Properties of total phase flows (in the panel on the right).

The total flow rates are visualized in a bar graph, indicating the amounts of solids, liquid and gas flow rates (**Fig. 18**).

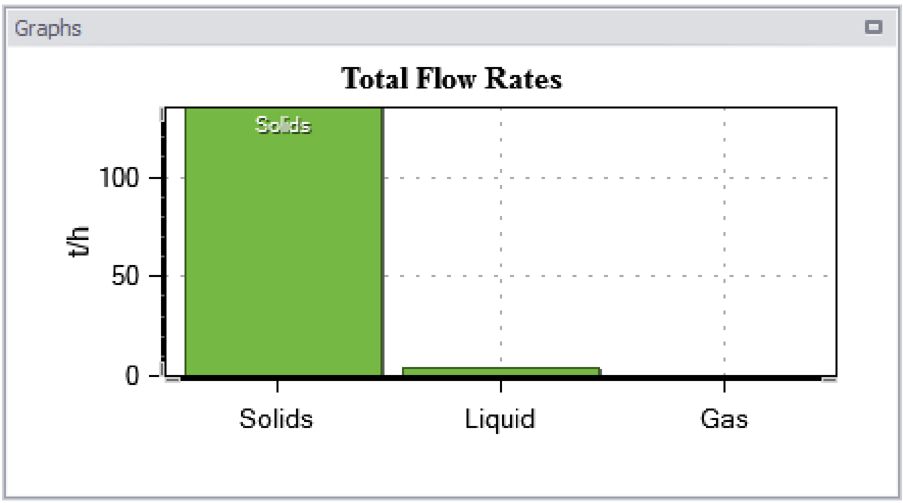


Fig. 18. Total flow rate graph.

45.3.1.2. Minerals

Minerals can be added by selecting them from the HSC Geo mineral database, or a new mineral can be created from scratch. In both cases the element composition as well as the specific gravity can be edited freely. The upper bar buttons for setting up the minerals are shown in **Fig. 19**.

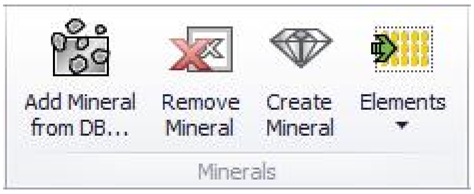


Fig. 19. Buttons for adding minerals from the database, removing minerals, creating new custom minerals, and editing their elemental composition.

- ✓ To open the HSC Geo **Select Mineral**s tool, click Add Mineral from DB...
- ✓ You can search for the mineral from the database; once the selected list is ready, click OK to accept (**Fig. 20**).

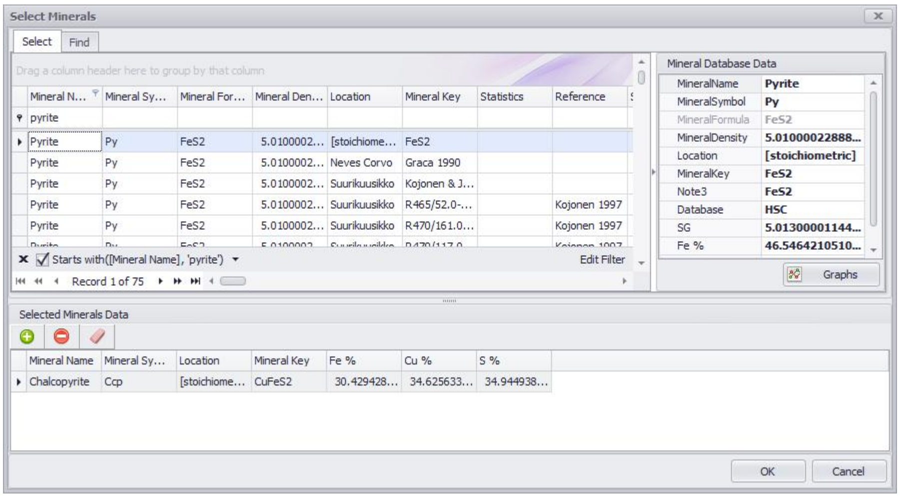


Fig. 20. Selecting minerals from the database.

Once the minerals are added, they will appear on the list, where the name, code, S.G., and formula can be edited (**Fig. 21**). The element composition of the minerals is presented in the lower part of the display, in the **Mineral Matrix** (**Fig. 22**).

Mineral	Code	S.G.	Formula	DB Ref.
Chalcopyrite	Ccp	4.35	CuFeS2	M/Ccp/40
Pyrite	Py	5.01	FeS2	M/Py/54
Quartz	Qtz	2.65	SiO2	M/Qtz/41

Fig. 21. List of selected minerals.

The Mineral Matrix allows you to edit the list of included elements; new elements can be added simply by typing them on the list and/or editing the existing elements. In the same way, the element wt% in each mineral can be edited.

Note I: the element wt% in each mineral is typically approximately 100%. However, this is not necessary; the chemical composition of a mineral can present just the measured elements for example.

Note II: the editing of the mineral properties (element wt%, S.G., etc.) does not affect them on the HSC Geo database. The edited minerals properties are only applied in the current HSC Sim simulation feed stream.

B2 34.6256332397461

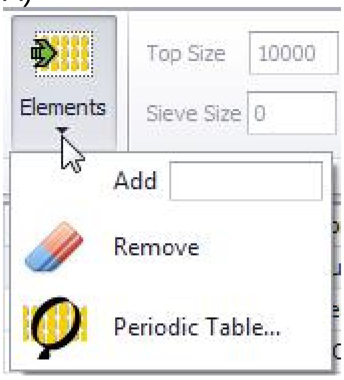
	A	B	C	D
1	Element	Ccp	Py	Qtz
2	Cu	34.63		
3	Fe	30.43	46.55	
4	O			53.26
5	S	34.94	53.45	
6	Si			46.74
7	Zn			
8				
9				

Mineral Matrix

Fig. 22. Mineral matrix for presenting and editing the element compositions of selected minerals.

Alternatively, to edit the Mineral Matrix element list in the lower part of the dialog, elements can be added, removed, or selected from the periodic table on the Elements button menu, shown in **Fig. 23**.

A)



B)

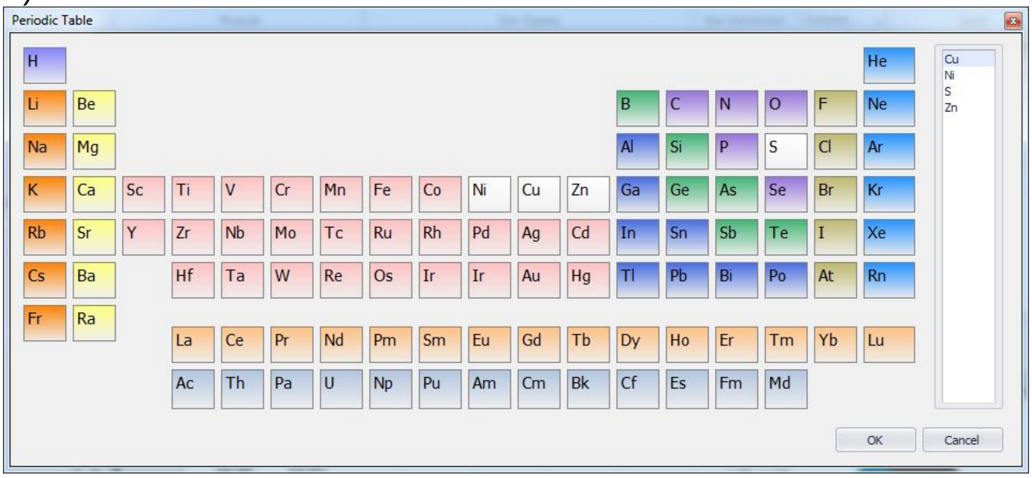


Fig. 23. Editing of elements, and selecting them from the periodic table.

The selected mineral (**Fig. 21**) properties are presented on the properties panel on the right (**Fig. 22**), and its element composition is presented visually in a pie chart (**Fig. 25**).

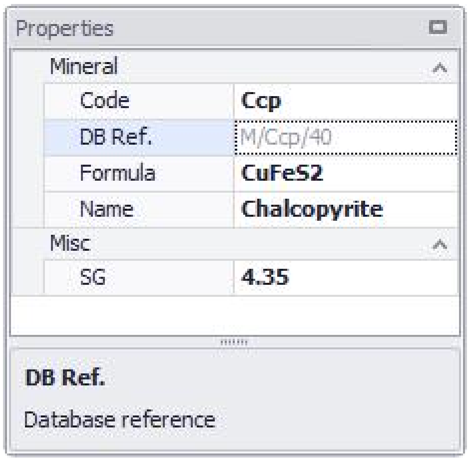


Fig. 24. Mineral properties.

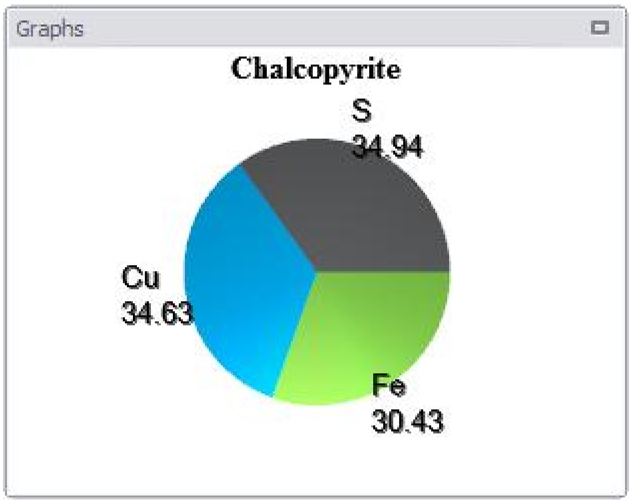


Fig. 25. Graphical presentation of the elemental composition of a mineral.

45.3.1.3. Size classes

The sieve size classes can be set up and edited as follows (**Fig. 26**):

- ✓ **Top Size** can be given or left empty; this affects the way the mean size of the topmost class is calculated
- ✓ **Sieve Size** is given and accepted by pressing Enter or the **Add Sieve** button (**Fig. 26**); alternatively there is a right mouse button tool for this (**Fig. 27**)
- ✓ The selected sieve can be removed by clicking **Remove Sieve**; or by right-clicking (**Fig. 27**)
- ✓ **Create Sieve Series** offers a way to create standard sieve series up to the given **Top Size** by using (**Fig. 28**):

- ISO 565 Test Sieves
- American Standard (ASTM E11)
- British Standard (BS 410)
- Square root of 2 series (down to > 1 µm)
- OR to create a given number of square root 2 series classes (up from 1 µm). In this case, Top Size is not needed.

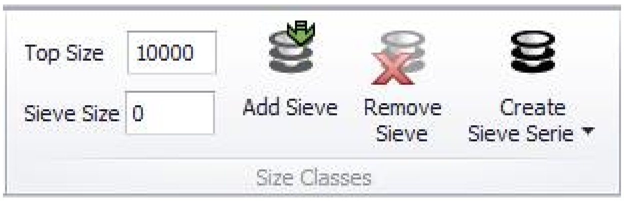
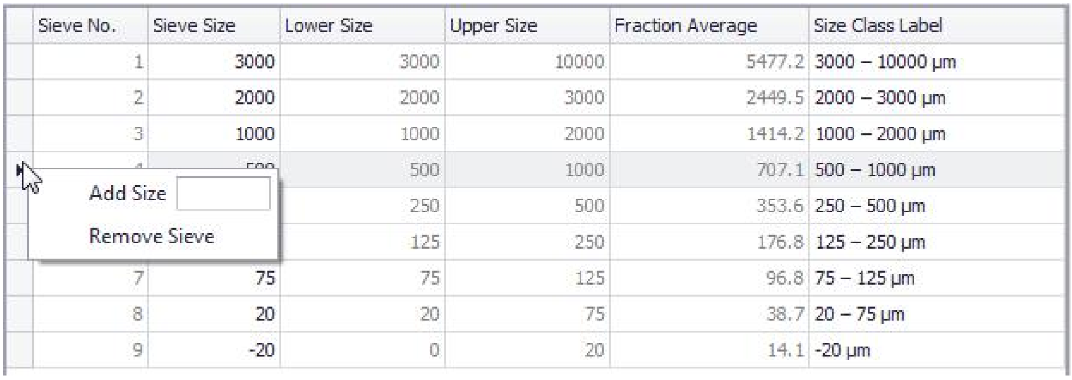


Fig. 26. Tool for creating and editing sieve size classes.



Sieve No.	Sieve Size	Lower Size	Upper Size	Fraction Average	Size Class Label
1	3000	3000	10000	5477.2	3000 – 10000 µm
2	2000	2000	3000	2449.5	2000 – 3000 µm
3	1000	1000	2000	1414.2	1000 – 2000 µm
4	500	500	1000	707.1	500 – 1000 µm
		250	500	353.6	250 – 500 µm
		125	250	176.8	125 – 250 µm
7	75	75	125	96.8	75 – 125 µm
8	20	20	75	38.7	20 – 75 µm
9	-20	0	20	14.1	-20 µm

Fig. 27. Size classes view for editing sieves and size class labels.

Fig. 28. Creating of a predefined sieve series.

Both the size class and size distribution properties are summarized on the right-hand panel (**Fig. 29**).

***<u>The user-editable values in Properties are</u>*:**

<u>Size Classes:</u>

- ✓ Select whether the size class labels are generated automatically or edited manually in the size class list (**Fig. 27**). These labels can be used in the unit models when you need to enter model parameters by size
- ✓ Measurement unit: µm or mm, this affects how the size data is shown in the Stream Setup tool, but for stream particles, the base unit for size is always the micrometer
- ✓ Top size, can be given or left empty

<u>Size Distribution:</u>

- ✓ Type: user-given size assay data or automatically generated distribution based on Rosin-Rammler or Gaudin-Schuhmann equations
- ✓ Rosin-Rammler equation parameters: a = 63.2 % passing size, b = distribution slope.
- ✓ Gaudin-Schuhmann equation parameters: k = 100% passing size, m = distribution slope.

***<u>The calculated values and information presented in the Properties are</u>* <u>(Fig. 29):</u>**

<u>Size Classes:</u>

- Number of size classes
- Indication if the feed is Unsized (bulk) or Sized
- Indication if the Top Size is given

<u>Size Distribution:</u>

- Calculated 50% passing size, P50
- Calculated 80% passing size, P80

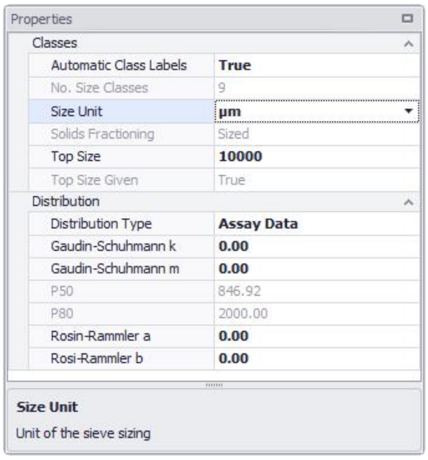


Fig. 29. The size class and size distribution properties.

45.3.1.4. Size distribution

The size distribution is given as wt% retained values for each size; the last size class is automatically calculated to total 100% (**Fig. 30**). Also, the cumulative passing % values are calculated automatically. Negative values are not allowed, and are indicated by red color, which must be corrected before proceeding further. If, instead of Assay Data (user-given values), the Rosin-Rammler or Gaudin-Schuhmann distribution calculation is selected (**Fig. 29**), the wt% values in **Fig. 30** will also be generated automatically.

Sieve No.	Sieve Size	Weight Retained (%)	Cumulative Passing (%)	Size Class Label
1	3000	8.9	91.1	3000 – 10000 µm
2	2000	11.1	80.0	2000 – 3000 µm
3	1000	24.7	55.3	1000 – 2000 µm
4	500	22.2	33.1	500 – 1000 µm
5	250	14.9	18.2	250 – 500 µm
6	125	8.7	9.6	125 – 250 µm
7	75	3.7	5.9	75 – 125 µm
8	20	4.3	1.6	20 – 75 µm
9	-20	1.6		-20 µm

Fig. 30. Defining the size distribution.

The size distribution (either Rosin-Rammler or Gaudin-Schuhmann) can be calculated in two ways:

1) By the equation, based on the two parameters given in Properties (**Fig. 29**)
2) By giving the known passing size value (e.g. for P80), the slope parameter is as given in Properties (**Fig. 29**), and the second parameter is solved by HSC Sim, by pressing Enter or clicking Calculate Distribution from the **Set Passing Size** button menu, shown in **Fig. 31**.

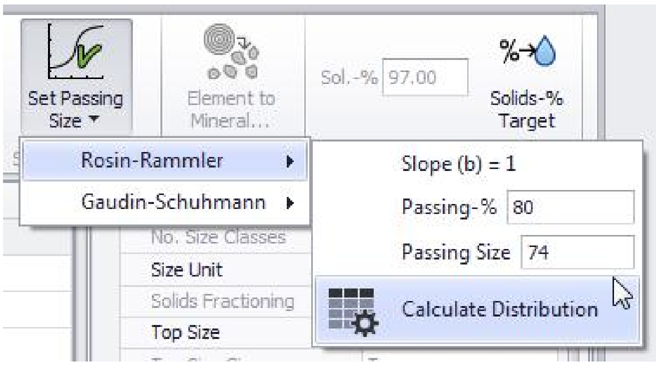


Fig. 31. Automatic calculation of the size distribution to match the given passing size value.

Finally, the cumulative size distribution curve can be seen graphically (**Fig. 32**). The figure includes both data points for each given sieve size and the quadratic spline interpolation curve between them.

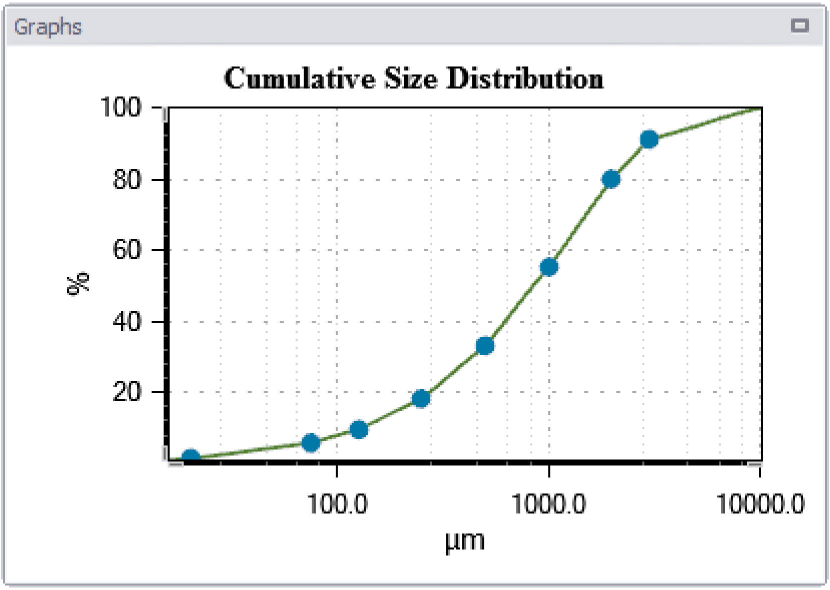


Fig. 32. Logarithmic presentation of the cumulative passing size; both the given sieve size data points and quadratic spline interpolation between them.

45.3.1.5. Mineral and elemental composition

The mineral compositions and resulting elemental compositions are edited from the tables shown in **Fig. 33**. The tables consist of:

<u>Mineral Composition:</u>

- Σ = 100: one of the minerals is always calculated as 100 % - the sum of all the other minerals
- Mineral: list of minerals (Codes)
- Bulk: bulk composition (cannot be edited when sized data; is then calculated automatically)
- Unit: %
- Size fractions: mineral composition of the fractions

Elemental Composition:

- Analyzed: indicates if the value is analyzed, thus it will not be updated based on the minerals. Instead, this is then the initial data for *element to mineral conversion*

- Element: list of all elements
- Bulk: bulk composition (cannot be edited when sized data, is then calculated automatically), editable for ‘Analyzed’ elements in the case of unsized data
- Unit: %
- Size fractions: elemental composition of the fractions. These are automatically calculated based on the minerals, except if the element is marked ‘Analyzed’ → will be the initial data for *element to mineral conversion*

F3 12.6263408131342

Σ = 100	Mineral	Bulk	Unit	-20 µm	20 – 75 µm	75 – 125 µm	125 – 250 µm
☐	Ccp	2.277274	%	1.0686	2.8302731	3.78332431	1.992743339
☐	Py	26.11407	%	21.564	25.276068	43.547916	21.89495501
☑	Qtz	71.60866	%	77.368	71.893659	52.6687597	76.11230165

Mineral Composition

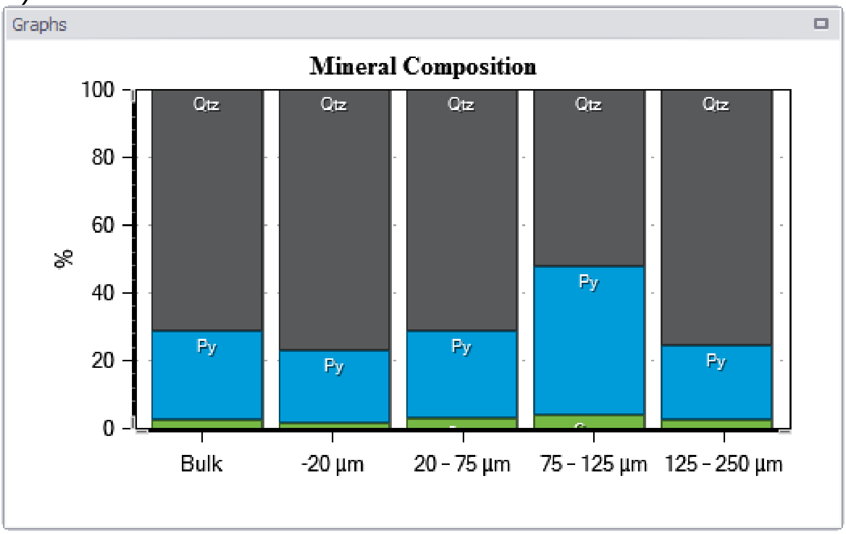
Analyzed	Element	Bulk	Unit	-20 µm	20 – 75 µm	75 – 125 µm	125 – 250 µm
☑	Cu	0.78852	%	0.37	0.98	1.31	0.69
☐	Fe	12.84813	%	10.362	12.626341	21.4212403	10.79769835
☐	O	38.13627	%	41.203	38.288052	28.0495422	40.53475392
☑	S	14.7547	%	11.9	14.5	24.6	12.4
☐	Si	33.47239	%	36.164	33.605607	24.6192176	35.57754773

Elemental Composition

Fig. 33. Mineral and elemental composition tables.

When the tables (shown in **Fig. 33**) are clicked, a graph will show either the mineral or elemental composition by size, see **Fig. 34**.

A)



B)

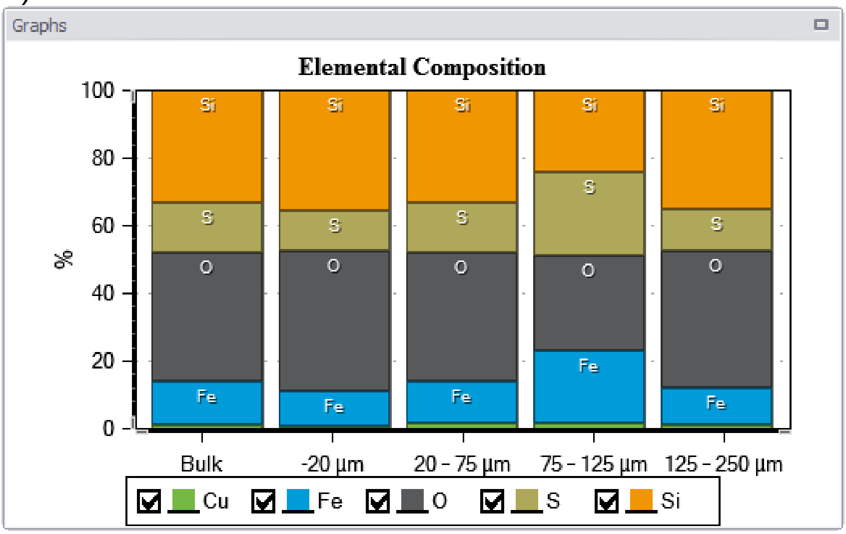


Fig. 34. Bar graphs of A) mineral and B) elemental stream composition for bulk and each size class.

A) Setting mineral composition – elements are calculated

The mineral composition can be simply entered in the upper table by each size class. One of the minerals is always selected, with **Σ = 100**, to be calculated as 100% minus all the other minerals (**Fig. 35**). The elements are automatically calculated and updated, but only if they are not marked **Analyzed**. The analyzed elements are the initial values for *element to mineral conversion* – explained in B).

1.06857251515991

A	B	C	D	E	
Σ = 100	Mineral	Bulk	Unit	-20 µm	20 -
☐	Ccp	2.277274	%	1.0686	2.8
☐	Py	26.11407	%	21.564	25
☑	Qtz	71.60866	%	77.368	71

Fig. 35. Entering the mineral wt% and selecting the Σ = 100 mineral.

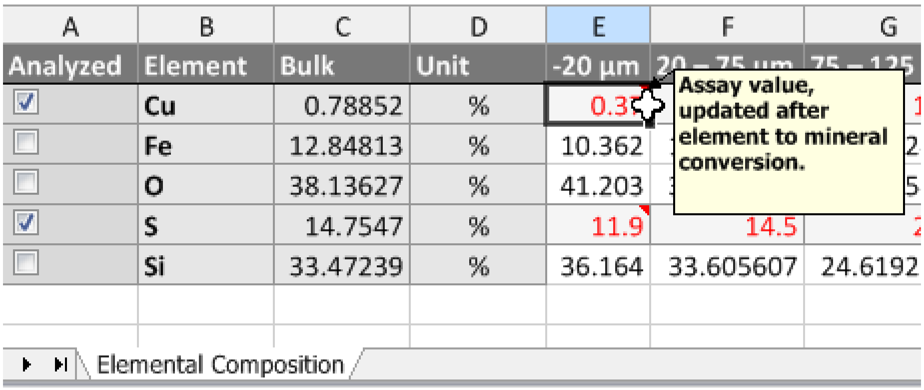


Fig. 36. Analyzed elements, not calculated from minerals, but updated after element to mineral conversion.

B) <u>Setting element composition – minerals are calculated</u>

Firstly, select the analyzed elements (**Fig. 36**); these are the initial values for element to mineral conversion. The conversion is done using HSC Geo in its **Modal Calculations** tool. To open HSC Geo for modal calculation, click the ‘**Element to Mineral...**’ button. The Modal Calculations dialog shown in **Fig. 37** will open.

The Modal Calculations tool indicates the selected elements in the periodic table and lists the minerals included in the Stream Setup. The calculation procedure is described in Chapter 84; in brief the steps are:

- ✓ Select the mineral(s) for calculation round 1
- ✓ Select the elements(s) for calculation round 1
- ✓ Add new calculation round(s) using the (+) ‘Add Round’ button
- ✓ The last round is practically always marked ‘Sum = 100 %’, thus that mineral is to be the remaining gangue material
- ✓ All the calculation rounds are then performed sequentially, with the selected method when you click ‘Calculate’
- ✓ When mineral composition calculation results are satisfactory, they are brought to Stream Setup by clicking ‘Update and Close’

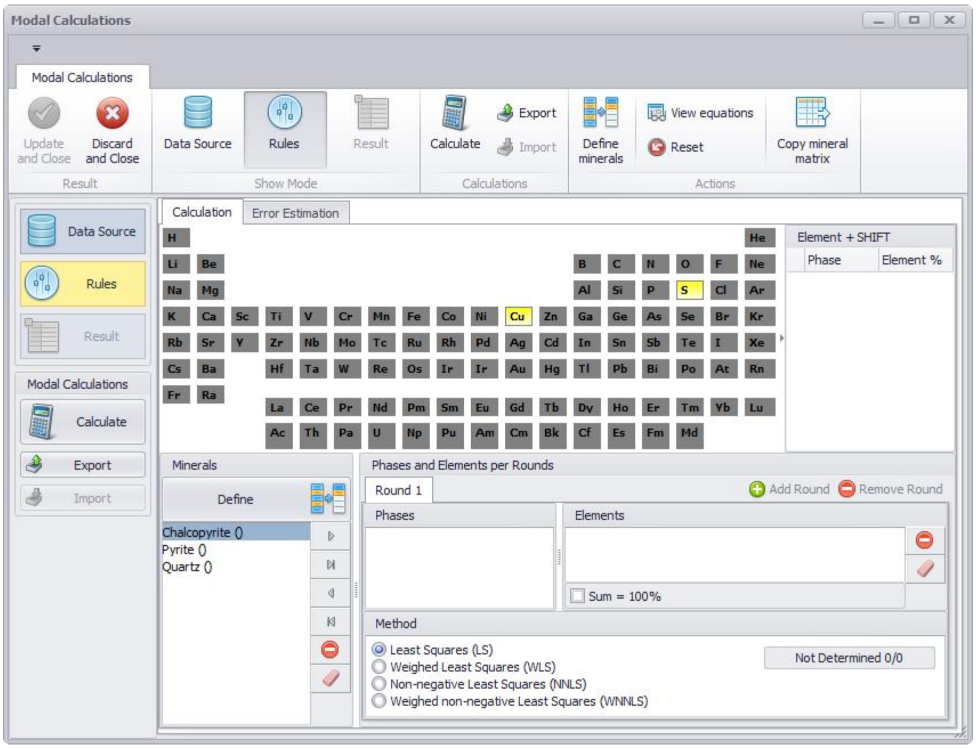


Fig. 37. HSC Geo Modal Calculations

When the element to mineral calculation with HSC Geo is ready, the results are seen in the Stream Setup Composition view, **Fig. 38**. Now, the tooltip of the ‘Analyzed’ values shows the original assay value, and the difference from it. The value in the corresponding cell shows the element wt% obtained in the mineral to element back calculation with the HSC Geo Modal Calculation tool.

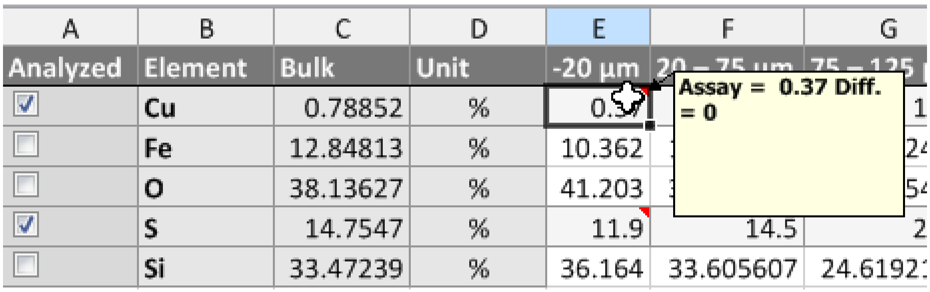


Fig. 38. Elements back-calculated from the minerals, after modal calculation in HSC Geo.

45.3.2. Liquid feed

The total liquid flow rate and its unit can be set in the Total Liquid Flow Rate view, see **Fig. 40**. Also, the liquid flow rate can be automatically calculated and kept updated, based on the given solids flow rate and solids percentage (**Fig. 39**), when the ‘**Solids % Target’** button is held down. Otherwise the ‘Sol. %’ text field indicates the calculated solids percentage based on the given solids and liquid flow rates.

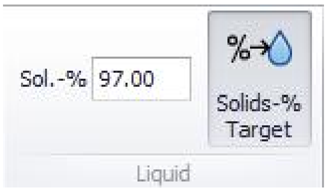


Fig. 39. Solids % target value for calculating the required liquid t/h

Phase Total	Amount	Unit
Liquid flow rate	4.18	t/h

Fig. 40. Total liquid flow rate.

45.3.3. Gas feed

The total gas phase flow rate is set from the Amount field shown in **Fig. 41**.

Phase Total	Amount	Unit
Gas flow rate	3.8	t/h

Fig. 41. Total gas total flow rate.

45.4. Selecting unit models

The unit models are selected for the unit icons of the flowsheet by using the Select Unit Models tool **Fig. 43**, which can be opened by:

- ✓ HSC Sim menu bar: Tools → Select Unit Models
- ✓ Right-clicking the unit (**Fig. 42**)
- ✓ Double-clicking the unit

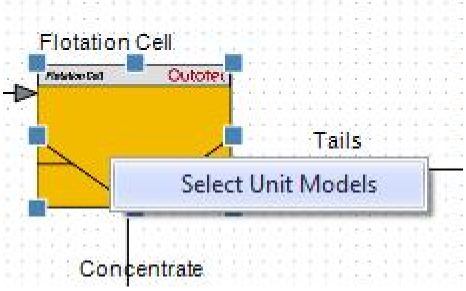


Fig. 42. Selecting a unit model for a unit.

The unit models are selected from the model library simply by double-clicking the model which is then assigned to the selected unit(s), **Fig. 43**. All the HSC Sim minerals processing unit models are shown under the Particles tab on the model list. The Select Unit Models dialog is also described in Chapter 40 (section 40.2.2.).

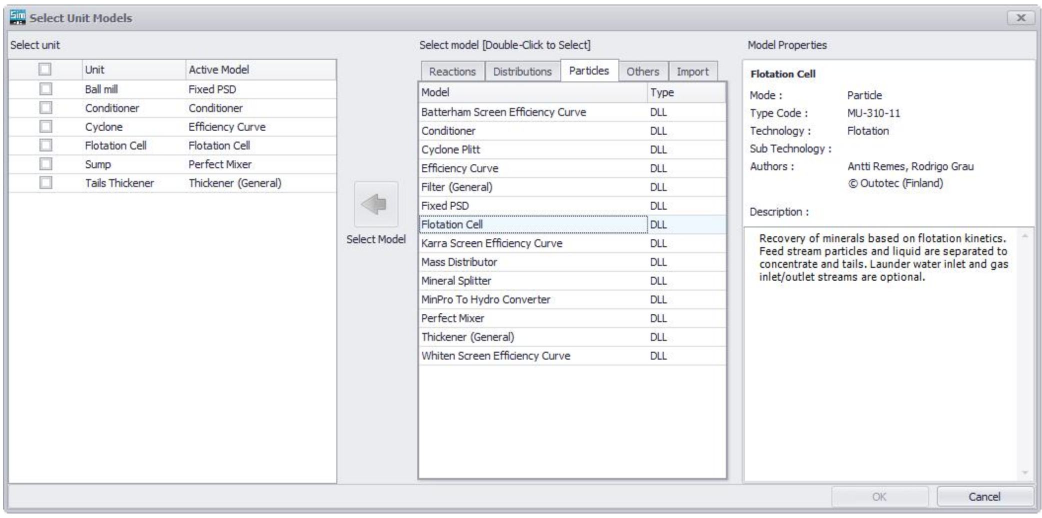


Fig. 43. Select Unit Models.

Once the models have been applied to the units, the model parameters are next edited and viewed with the model editor as shown in **Fig. 44**. The model input and output streams can be viewed, their connection to the model inputs and outputs can be configured, and controls for the models can be defined.

Setting up the **Controls** and **Cell References** between the units is described in sections 43.5. and 44.2.5.

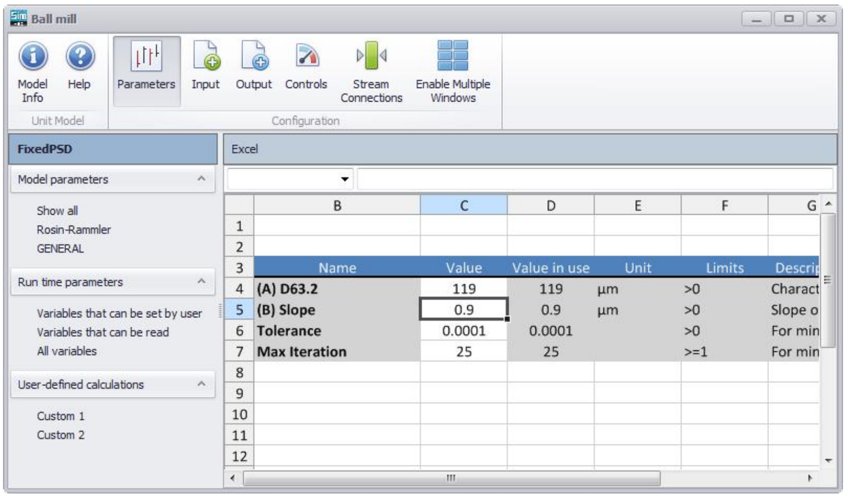


Fig. 44. Dialog to enter and view the unit model parameters, stream content, stream connections, and model controls.

45.5. Run simulation and view the results

45.5.1. Simulate

To run the simulation from the HSC Sim upper bar buttons (**Fig. 45**):

- ✓ Set the number of calculation rounds. This is how many sequential calculations are repeated through all the units.
- ✓ Click the ‘Simulate’ button
- ✓ If the flowsheet is not yet in balance (stream content is still changing round by round), repeat the simulation; you may also increase the number of calculation rounds

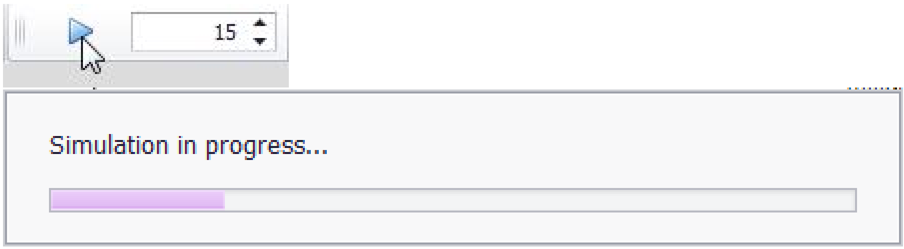
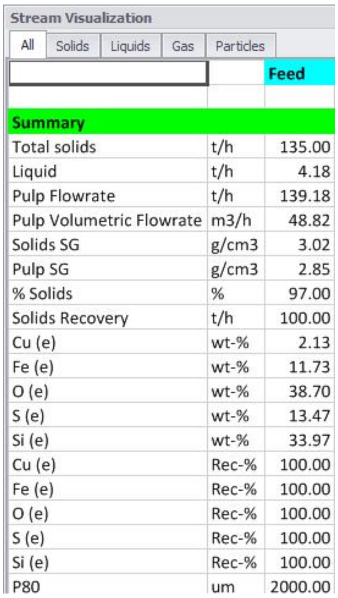


Fig. 45. Simulating the process.

45.5.2. Visualization, tables, graphs, scenarios

In the Visualization mode  the stream content and listing of all the variables calculated from the particles can be seen with the Stream Viewer (**Fig. 46**). A mineral processing stream consists of the following variables:

- Total solids, t/h
- Liquid, t/h
- Pulp flow rate, t/h
- Pulp volumetric flow rate, m^3/h
- Solids SG, g/cm^3
- Pulp SG, g/cm^3
- % Solids
- Solids recovery %
- Element wt%
- Elements recovery %
- Mineral wt%
- Mineral recovery %
- Passing sizes, P50 and P80 µm
- Size fraction percentages %



Stream Visualization

All | Solids | Liquids | Gas | Particles

		Feed
Summary		
Total solids	t/h	135.00
Liquid	t/h	4.18
Pulp Flowrate	t/h	139.18
Pulp Volumetric Flowrate	m3/h	48.82
Solids SG	g/cm3	3.02
Pulp SG	g/cm3	2.85
% Solids	%	97.00
Solids Recovery	t/h	100.00
Cu (e)	wt-%	2.13
Fe (e)	wt-%	11.73
O (e)	wt-%	38.70
S (e)	wt-%	13.47
Si (e)	wt-%	33.97
Cu (e)	Rec-%	100.00
Fe (e)	Rec-%	100.00
O (e)	Rec-%	100.00
S (e)	Rec-%	100.00
Si (e)	Rec-%	100.00
P80	um	2000.00

Fig. 46. Stream Viewer for inspecting the stream content

Values that are shown on the flowsheet stream value labels are selected from the HSC Sim main window dropdown menu, see **Fig. 47**. The same values are also used for the Sankey diagram, presenting the value with the flowsheet stream line width.

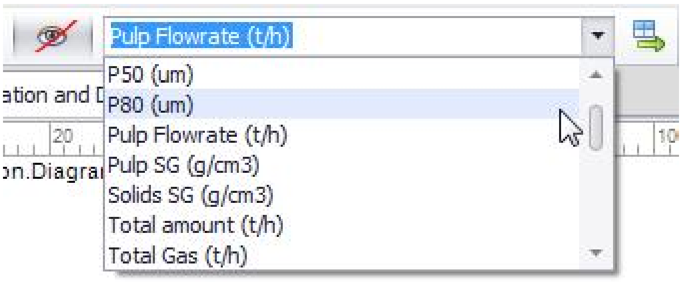


Fig. 47. Stream Visualization to set the values to be shown on the stream value labels and stream Sankey diagram (line width).

In addition, the variables can be shown on the flowsheet in tables. The variables can be inserted and edited with the Stream Table Editor (**Fig. 48**); see section 40.1.4. Tables can also be inserted from Tables button on the left (**Fig. 49**) and by editing the content manually with cell reference and text.

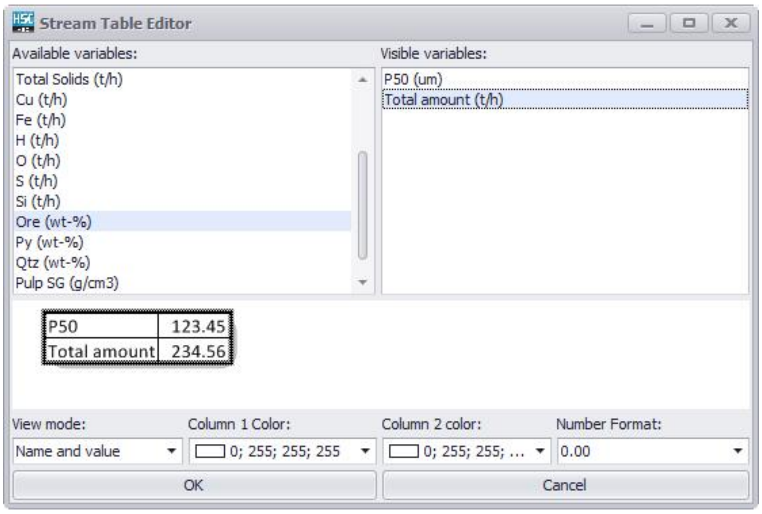


Fig. 48. Stream Table Editor for adding tables that present the stream variable details.

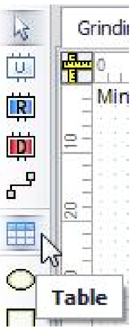


Fig. 49. Inserting tables from the left-bar button Table selection.

It is also possible to repeat a sequence of simulations with different model parameterization and/or feed composition, and record the simulation results (**Fig. 50**). This can be done by selecting:

- ✓ HSC Sim menu bar: Tools → Run Scenarios

This will open the Scenario Editor described in section 40.2.3.

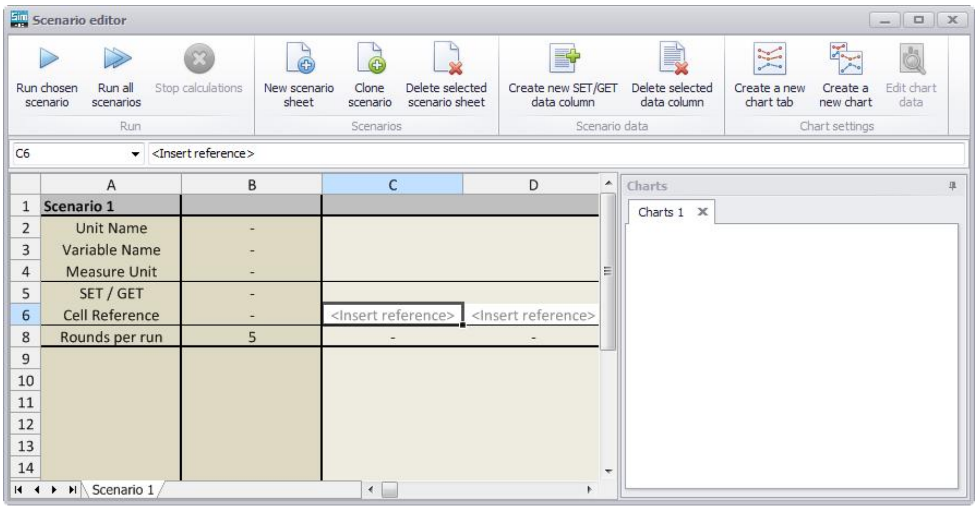


Fig. 50. Scenario Editor, for running different simulation set-ups and recording the simulated values.

45.6. Opening an HSC 7 flowsheet in HSC 8

The old HSC 7 flowsheet can be opened, simulated and edited, albeit with some restrictions, in HSC 8. The steps for handling HSC 7 flowsheet models are described briefly in the following section.

45.6.1. Conversion from HSC 7 to HSC 8 format

When a HSC Sim 7 flowsheet model (.fls file) is opened, HSC Sim 8 will convert it into the new format (**Fig. 51**). For a large flowsheet, this may take several minutes. For more details about importing, see Chapter 40 (section 40.4.).

Fig. 51. Importing an HSC 7 flowsheet.

When the importing is ready, save the model in a new separate folder.

45.6.2. Simulating the flowsheet

The HSC 7 imported models are simulated in a similar way, by setting the number of calculation rounds and clicking ‘Simulate’ (**Fig. 45**). If some errors or warning occur, please refer to Chapter 40 (section 40.4) for how to solve them.

45.6.3. Modifying feed composition

The feed composition can be edited by selecting from the HSC Sim menu bar: Tools → Old Mineral Setup (visible only for imported models)

In Mineral Setup (**Fig. 52**) you can:

- ✓ Change the element wt% in each mineral
- ✓ Change the mineral SG
- ✓ Change the water SG
- ✓ Change the feed rate t/h
- ✓ Change the particle size distribution wt%
- ✓ Change the mineral composition by size
- ✓ Change the fraction amounts of floatability classes

But you cannot:

- Add, remove or rename minerals
- Add or remove elements
- Change the number of size classes
- Change the number of floatability classes

since they affect the variable list content, which can be edited only in HSC 7 for the old file format models.

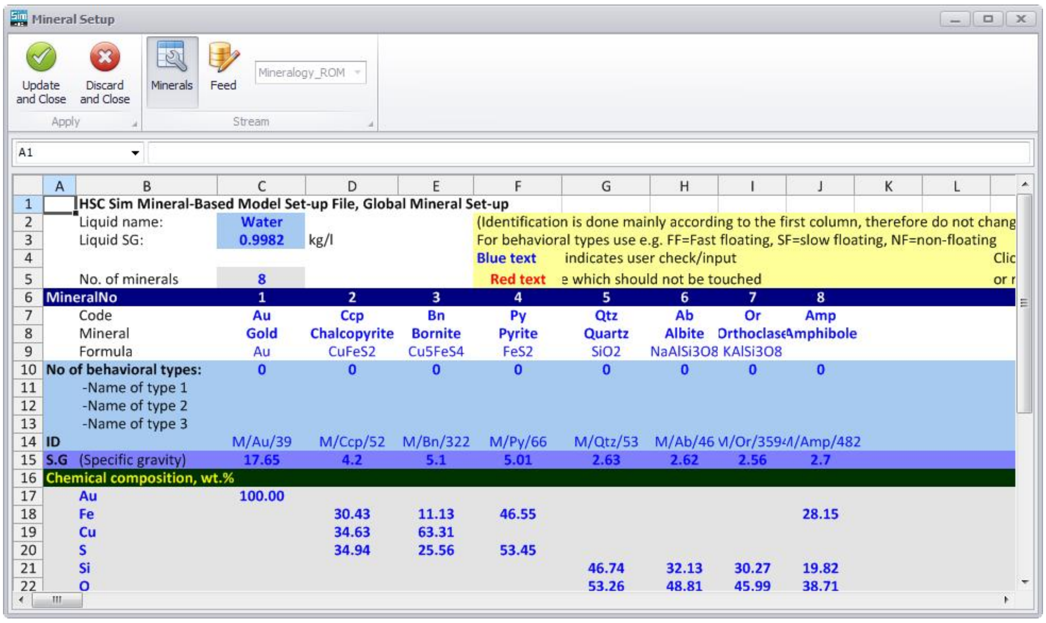


Fig. 52. Mineral Setup for HSC 7 imported models

45.6.4. Editing model parameters and reloading the unit models

Open the unit model editor by double-clicking the unit. It opens a similar view as in HSC 7 (**Fig. 53**), consisting of:

- Input: list of input streams of the units
- Output: list of output streams of the unit
- Dist: material distribution calculation form
- Control: model controls sheet
- Model: model parameters sheet
- Wizard: sheet containing the Excel Wizard initial data
- Other sheet: sheets that the model may contain, e.g. Tank

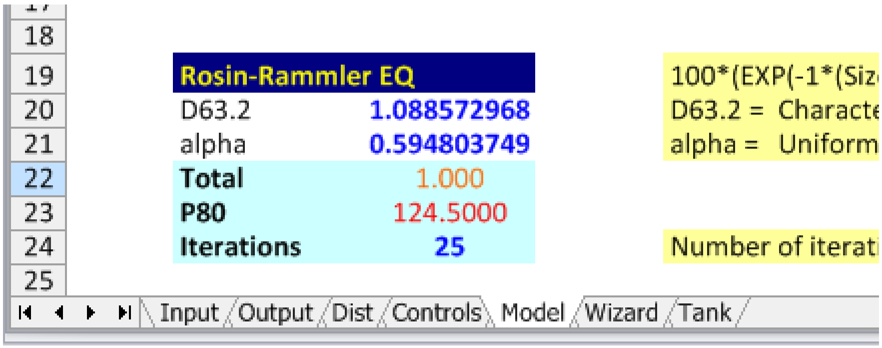


Fig. 53. Example of unit editor navigation tabs for HSC 7 imported models.

46. Sim Minerals Processing Unit Models

TOC:

46.1. Minerals Processing Unit Model Library

HSC Sim 8 includes a library of process models covering a wide range of unit operations in mineral processing. In HSC Sim the process models for the unit operations are called ***unit models*** while the process flowsheet calculation blocks are ***units***. All the calculations are performed using *solids*, *liquid,* and *gas* phases, where the solids are always defined as *mineral particles* for minerals processing applications. Thus the model calculations are performed with an HSC Sim ***Particles*** type model.

To define a feed stream for Particles models in HSC Sim, the ***Stream Set-up*** (see Chapter *45 Sim Minerals Processing*) tool is used. Mineral processing units can also be connected to other process unit model types (e.g. hydrometallurgical and pyrometallurgical units) by using the stream conversion block between them (see Chapter 47).

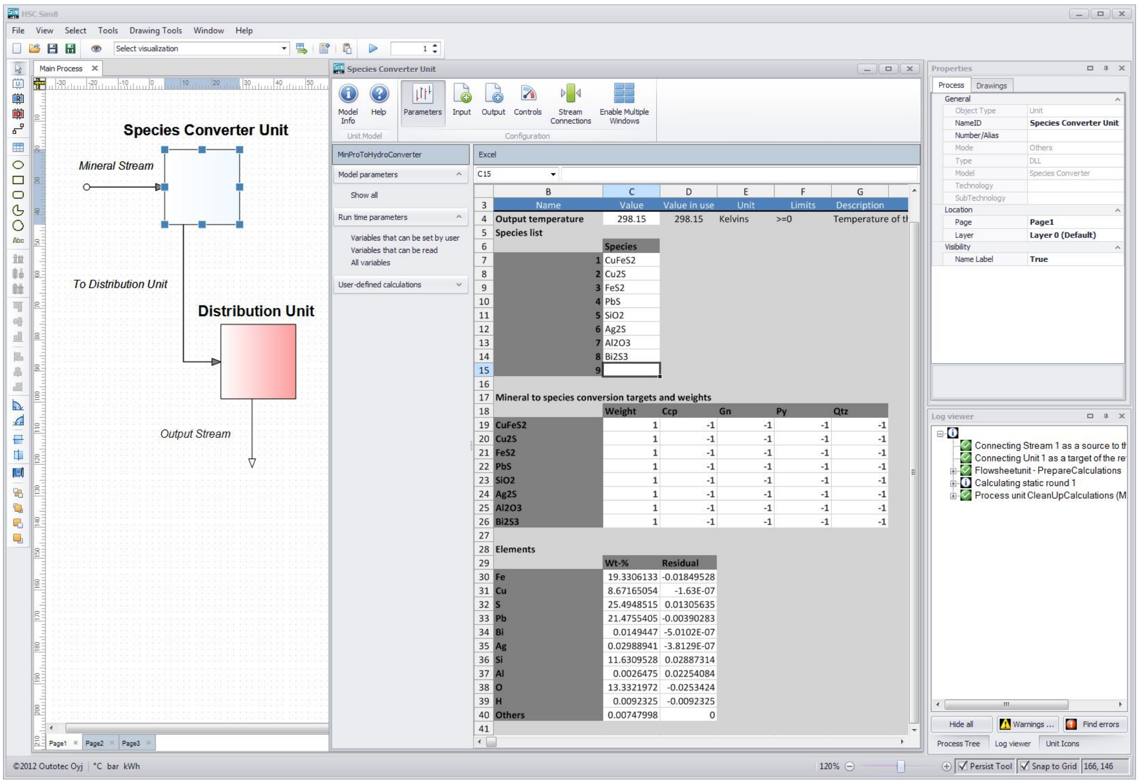
To create your own custom unit models, programmed as DLL files, please refer to Chapter 50.

Table 1 summarizes the HSC Sim minerals processing unit model library:

Table 1. HSC Sim minerals processing unit models.

Technology	Type Code	Model	Description
Concentrator General	MU-110-10	Perfect Mixer	Mixes all input material from one or several streams and passes it equally to one or several outputs
Separation General	MU-120-10	Efficiency Curve (Whiten)	Whiten efficiency curve. Supports separation by mineral and inclusion of the 'fish-hook' effect
	MU-120-11	Mass Distributor	Distributes solids and water to several outputs with given ratios
	MU-120-12	Mineral Splitter	Mineral by size split of the feed into the concentrate and tails streams, and optionally into a middlings stream
Comminution General	MU-130-10	Fixed PSD (Rosin-Rammler)	Fixed Particle Size Distribution, calculated by using Rosin-Rammler or Gaudin-Schuhmann equations
Screens	MU-230-10	Whiten Efficiency Curve	Whiten screen efficiency curve
	MU-230-11	Karra Efficiency Curve	Karra screen efficiency curve
	MU-230-12	Batterham Efficiency Curve	Batterham screen efficiency curve
Hydrocyclones	MU-240-10	Plitt	Separation in hydrocyclone according to the Plitt model. Supports separation by mineral. Indicates if underflow discharge is roping
Flotation	MU-310-10	Conditioner	Conditioning of particles by setting the flotation kinetic parameters based on the selected calculation model. Recycle stream is directed through without changes in the kinetics
	MU-310-11	Flotation Cell	Recovery of minerals based on flotation kinetics. Feed stream particles and liquid are separated to concentrate and tails. Launder water inlet and gas inlet/outlet streams are optional
Thickeners	MU-510-10	Thickener (General)	General thickening model. Produces given underflow solids percentage and overflow water clarity
Filters	MU-520-10	Filter (General)	General filtering model. Produces given cake moisture and filtrate clarity, supports optional inlet/outlet streams for technical waters

47. Sim Species Converter Units



In Sim 8, it is possible to connect minerals processing DLL units to conventional Reactions(Hydro) and Distribution(Pyro) units. However, this connection requires that the content of the mineral streams is converted to chemical species. This conversion is carried out with the Species Converter unit.

47.1. Selecting the Species Converter unit model

The Species Converter unit model is selected with the "Select Unit Model" tool (**Fig. 1**). Mineral streams are connected as inputs, and the output of a Species Converter unit is connected either to a Reactions or a Distribution unit.

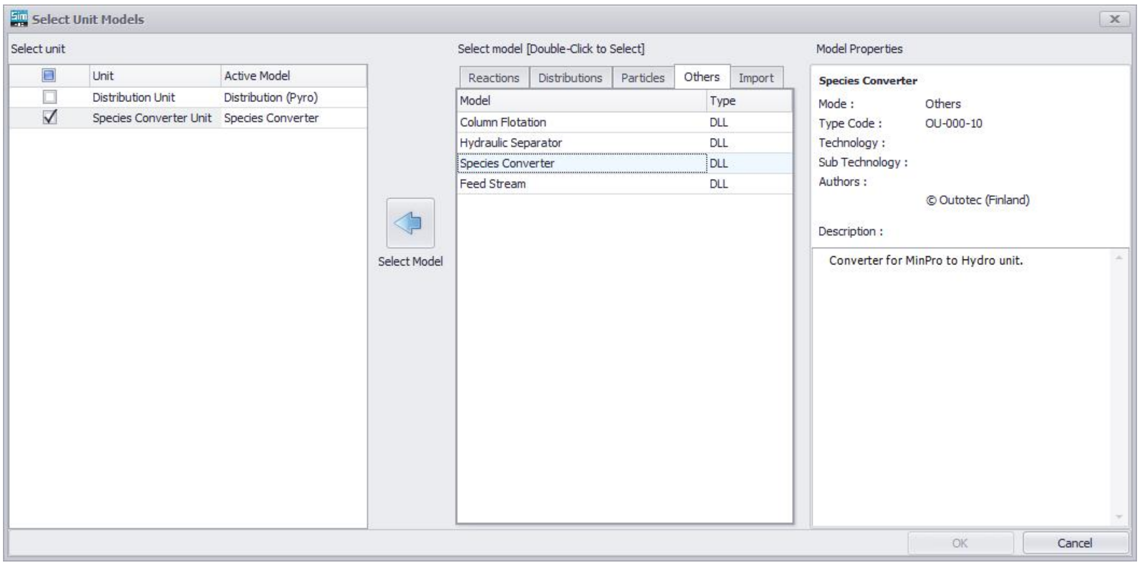


Fig. 1. Selecting the Species Converter unit model.

47.2. Setting the conversion parameters

The conversion, from the element distribution of the minerals to chemical species, requires a list of species. These species are entered on the "Parameters" page in the unit, under the "Species" heading (**Fig. 2**).

6		Species
7	1	CuFeS2
8	2	Cu2S
9	3	FeS2
10	4	PbS
11	5	SiO2
12	6	Ag2S
13	7	Al2O3
14	8	Bi2S3
15	9	

Fig. 2. Enter the species that can be formed.

Users can also set optional parameters for the conversion, to adjust the conversion by target values and weighting coefficients. These optional parameters are entered in the mineral-species matrix (**Fig. 3**). If a species does not have any specific target values, then "-1" is used as a default parameter.

17	Mineral to species conversion targets and weights					
18		Weight	Ccp	Gn	Py	Qtz
19	CuFeS2	5	80	0	0	0
20	Cu2S	1	-1	-1	-1	-1
21	FeS2	1	15	0	100	0
22	PbS	1	-1	-1	-1	-1
23	SiO2	10	0	0	0	100
24	Ag2S	1	-1	-1	-1	-1
25	Al2O3	1	-1	-1	-1	-1
26	Bi2S3	1	-1	-1	-1	-1

Fig. 3. Set target and weight coefficient values, to adjust the conversion.

Finally, when all the necessary parameters are set, run the model to get the conversion results.

47.3. Conversion results

After the model is run, the conversion results can be checked from the "Output" page to see the actual amounts of the species. However, it is also extremely important to check the element balance on "Parameters" page after the conversion, to ensure that the residuals of the element balance are acceptable (**Fig. 4**). If the residual values are too high, you can try to obtain a better conversion by adding more species to the list or by changing the target and weighting parameters.

28	Elements		
29		Wt-%	Residual
30	Fe	19.3306133	-0.01834455
31	Cu	8.67165054	-2.5977E-07
32	S	25.4948515	0.01318637
33	Pb	21.4755405	-0.00418113
34	Bi	0.0149447	-5.3151E-07
35	Ag	0.02988941	-4.089E-07
36	Si	11.6309528	0.02887313
37	Al	0.0026475	0.02254082
38	O	13.3321972	-0.02534243
39	H	0.0092325	-0.0092325
40	Others	0.00747998	0

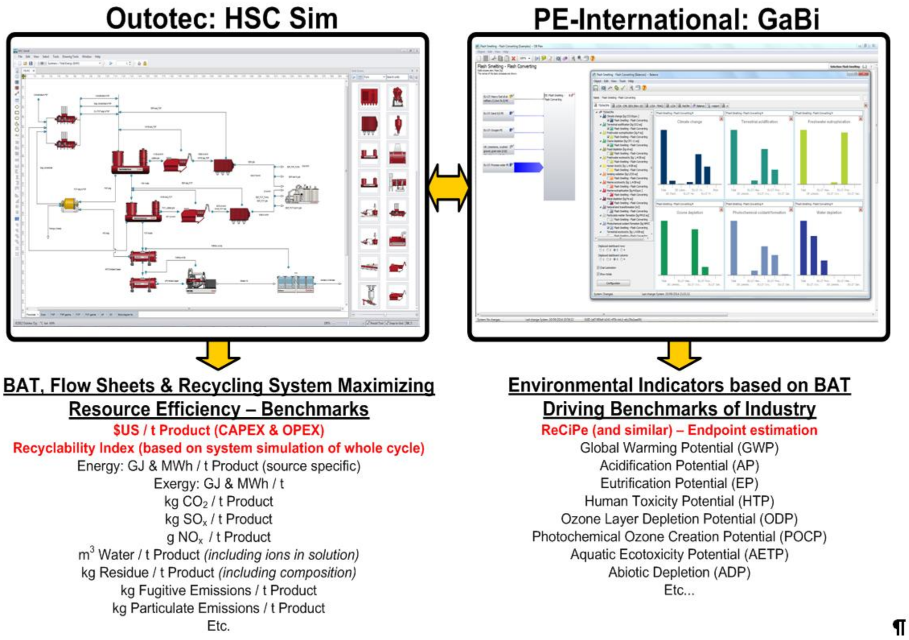
Fig. 4. Element balance residuals after conversion.

47.4. Advices when using Species Converter unit

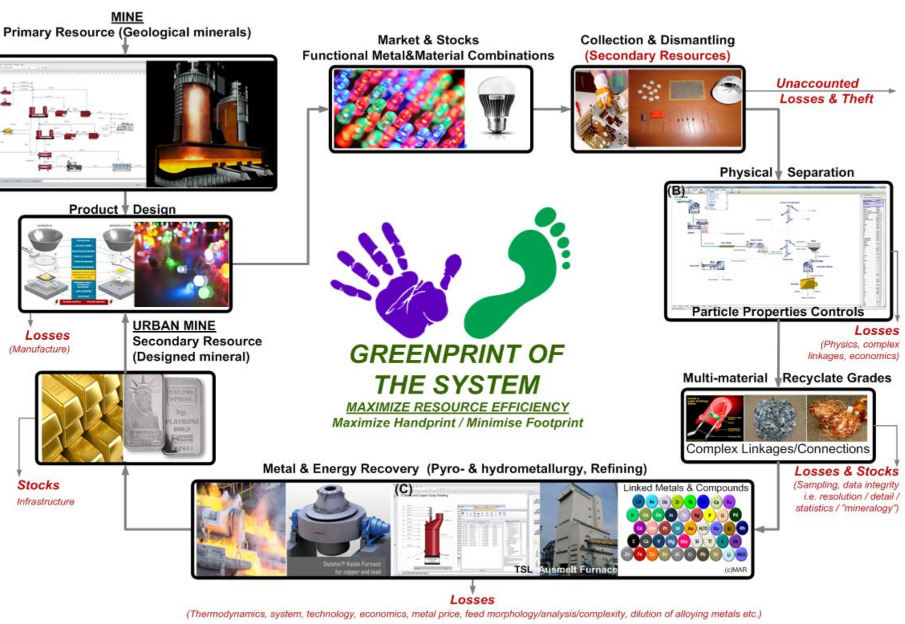
- The species used in the conversion have to be found from the active HSC database (main or own).
- Usually the more species is specified, the better conversion is obtained (small element balance residuals).
- H2O amount of the input mineral streams is automatically converted to the output stream.
- When connecting the output of a Species Converter unit to a Reactions(Hydro) unit, all the converted species have to be found from the variable list, including "Others".

49. Environmental Impact

Environmental impact assessment in HSC Sim 8 combines the simulation functionality of Sim with the functionality of GaBi environmental impact assessment software[1]. This provides a rigorous mass and energy balance as well as a techno-economic basis for LCA and thus links the environmental impact analysis to technology. Hence it can be used to suggest change and innovation.



All analyses are performed on this basis, linked to technology, and can therefore be used to innovate the technology and/or the system and understand its resource efficiency, as shown in **Fig. 1**.



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49.1. Introduction to Life Cycle Assessment (LCA)

Calculating a LCA is defined in the ISO 14040 and 14044 standards, which belong to the ISO environmental management standards family ISO 14000. According to the standards, the calculation is divided into the four main phases presented in **Fig. 1**.

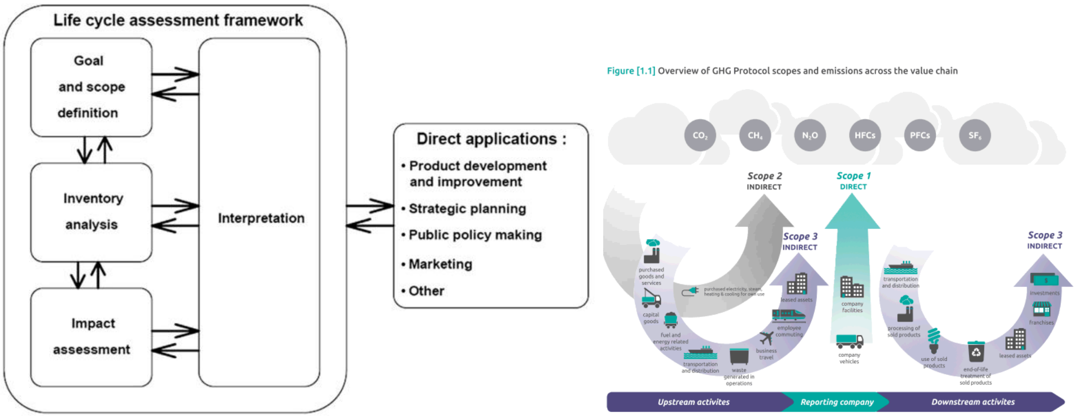


Fig. 1. Steps of Life Cycle Assessment[1-4] to capture Scope 1 to 3 emissions and impacts on the environment.

1. Goal and scope definition phase. In this 1st phase, system boundaries will be defined for the analyzed system. System boundaries define which Unit Processes (phases) will be included in the LCA.

   - Cradle to Grave (Full Life Cycle Assessment)
   - Cradle to Gate (Exclude transportation part to customer)
   - Gate to Gate (One process in the production chain)

   The depth and breadth of an LCA depend on the goal of each particular LCA. The reason for making the LCA and the target group usually define the goal of the LCA.

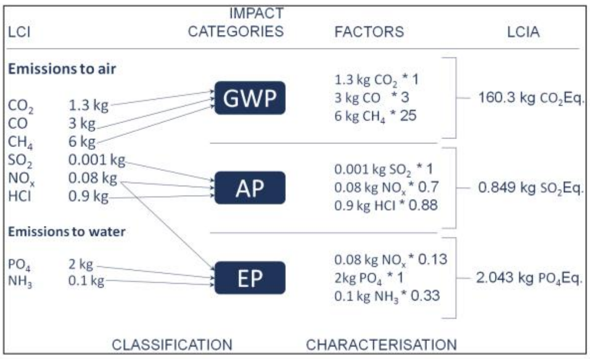
2. Inventory analysis phase. This phase is also called the Life Cycle Inventory (LCI) phase, which is the 2nd phase of LCA. This phase is usually the most time-consuming phase, where the input and output data regarding the system are studied and collected. LCI answers the question: How much of everything flows where?

   Usually input and output can be classified into the following main fields:

   - energy inputs, raw material inputs, ancillary inputs, other physical inputs
   - products, co-products, and waste
   - releases into air, water and soil, and
   - other environmental aspects.

   All calculating procedures should be explicitly documented and all assumptions should be explained carefully. It is good to check the data validity during the LCA process. A production flow definition should be made using the real production distribution. For example, in the case of electricity, details such as fuel combustion, mix, conversion, etc. should be included.

3. Impact assessment phase. The 3rd phase of LCA is also known as Life Cycle Impact Analysis (LCIA). LCI results allow you to calculate the LCIA of the system. LCIA identifies and evaluates the amounts and significance of the potential environmental impacts of the product system. LCIA answers the question: What are the resulting impacts? Calculating is usually done using four steps, where the first two are mandatory. **Fig. 2** describes the steps with example values.



Industrial designation or common name	Chemical formula	GWP for 100-year time horizon	
		Second assessment report (SAR)	4th assessment report (AR4)
Carbon dioxide	CO_2	1	1
Methane	CH_4	21	25
Nitrous oxide	N_2O	310	298
Substances controlled by the Montreal Protocol			
CFC-11	CCl_3F	3,800	4,750
CFC-12	CCl_2F_2	8,100	10,900
CFC-13	$CClF_3$		14,400
CFC-113	CCl_2FCClF_2	4,800	6,130
CFC-114	$CClF_2CClF_2$		10,000
CFC-115	$CClF_2CF_3$		7,370
Halon-1301	$CBrF_3$	5,400	7,140
Halon-1211	$CBrClF_2$		1,890
Halon-2402	$CBrF_2CBrF_2$		1,640
Carbon tetrachloride	CCl_4	1,400	1,400
Methyl bromide	CH_3Br		5
Methyl chloroform	CH_3CCl_3	100	146

Fig. 2. Life Cycle Impacts Analysis steps and a few impact factors for CO_2 Eq.

- Classification (All emissions are linked to one or more impact category), for example CH_4 belongs to the Global Warming Potential (GWP) category.

- Characterization (Converts reference substance of the category by multiplying the quantities by the characterization factor, which means that the result unit is changed to the reference unit of the category where the quantity belongs. For example, CH_4 has a factor of 25, which means that CH_4 contributes 25 times more than CO_2 to the global warming potential. The most common factor developers are the Institute of Environmental Science (CML) in Europe and TRAICI in the United States[3-4].

- Normalization (Converts and possibly aggregates the indicator results across impact categories using numerical factors based on value choices. The aim is to understand the relative magnitude for each indicator result.)

- Evaluation (Gives better understanding of the reliability of the collected indicator results. More like a quality control step.)

4. Interpretation phase. In this 4th and final phase of the LCA procedure, the results of the LCI or LCA or both, are summarized. The main idea here is to identify significant issues based on the LCI and LCIA phases of LCA.

Not all of these phases are always mandatory. Sometimes sufficient information is already assimilated by carrying out only the LCI and LCIA phases. This is usually referred to as an LCI study.

49.2. LCA in HSC Sim

The HSC Sim LCA tool covers LCA phases one and two. Subsequent phases are performed by 3rd party LCA software. When the LCI has been completed via HSC Sim, the process and/or flowsheet is/are exported to a separate file that can be imported into GaBi LCA software (the file is in Ecospold format). In GaBi software, other Scope 2 and 3 processes, transportation etc. are added, as will be shown in the example below. Please consult www.pe-international.com for more information and details about GaBi at http://www.gabi-software.com/.

The HSC Sim LCA tool can also be used to capture, in a black box summary, how much of a compound is released into the environment, without the use of GaBi software. However, GaBi provides mid- and end-point analyses of the impacts of these flows, materials, compounds etc. providing a detailed impact analysis of the flows.

HSC Sim LCA analysis is always based on a complete HSC Sim process model, where the input and output streams represent the data for the LCIA phase. In LCA analysis, the substances of interest are only the input and output streams to the environment. Internal streams are not taken into account because they are not relevant when analyzing the process as one black box. As LCA does not generally base its analysis of complete systems on closed mass and energy balances, it is always advisable to create a detailed process model to make the LCA results more accurate.

49.3. Using the LCA Tool in HSC Sim

When the process simulation model is ready, the LCA tool is started by selecting Tools → LCA Evaluation from the main menu as shown in **Fig. 3**.

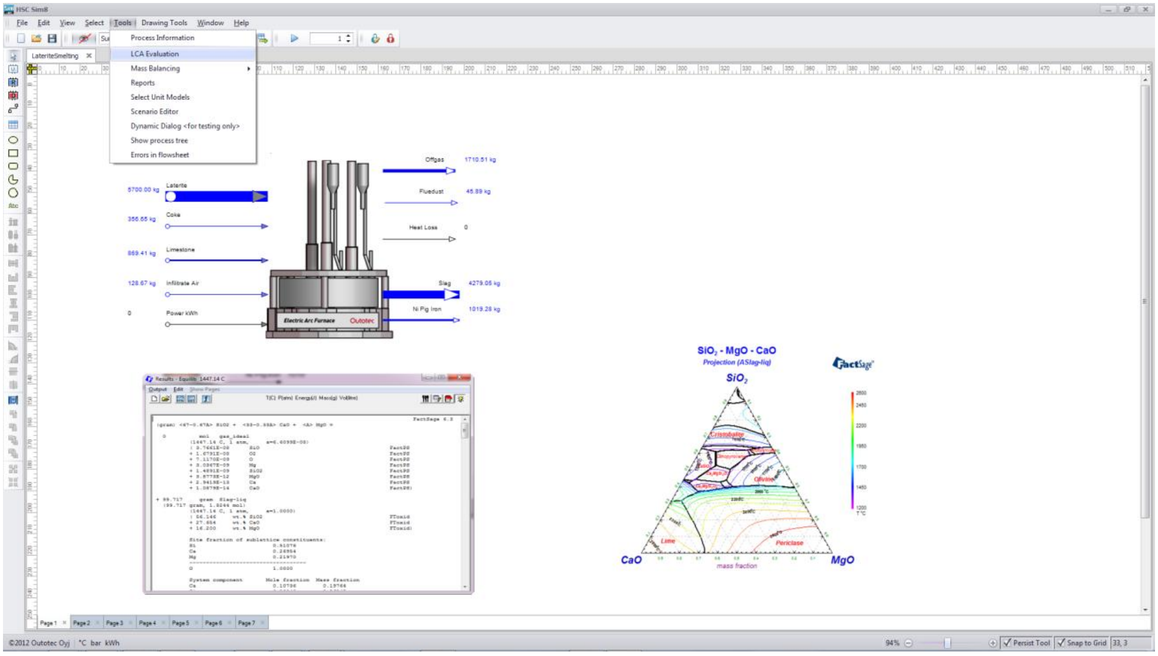
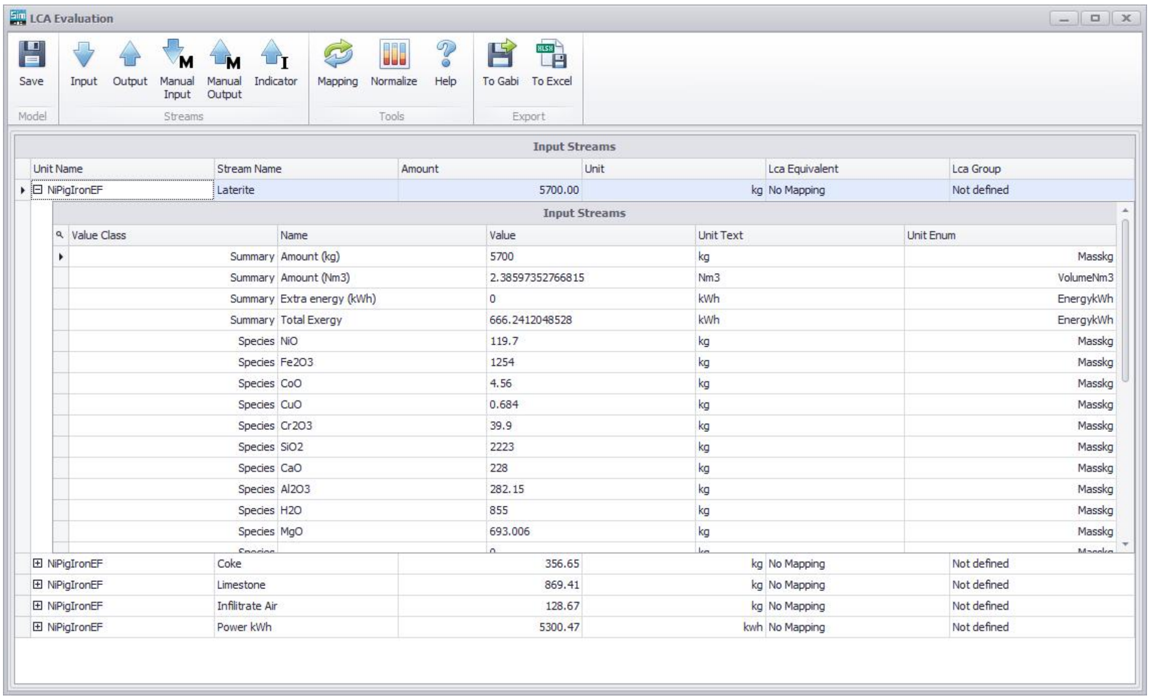


Fig. 3. Starting the LCA tool from the main menu, also showing a Sankey diagram for total mass flow and some extra information required for slag chemistry to check the results.

49.3.1. Automatic Import of All Input and Output Streams

The LCA tool creates up to five sheets, namely Input, Output, Manual Input, Manual Output, and Indicator as shown in **Fig. 4**. The Input and Output Streams Info sheets contain all the process input and output streams in HSC Sim format for the process or complete flowsheet. In these sheets, stream detail content is available and imported directly from the simulation model.

NOTE: No internal streams are captured through this, as only streams that can interact with the environment and flow out from the system into the environment are used in the assessment.



Unit Name	Stream Name	Amount	Unit	Lca Equivalent	Lca Group
NiPigIronEF	Laterite	5700.00	kg	No Mapping	Not defined

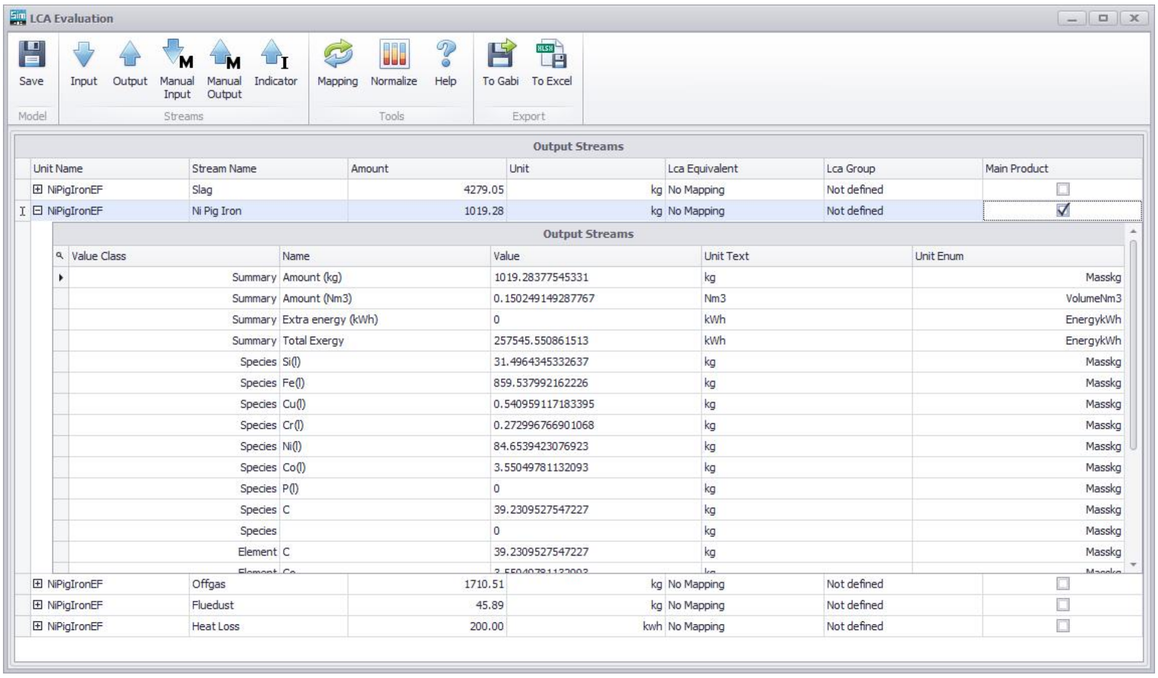
Input Streams

Value Class	Name	Value	Unit Text	Unit Enum
Summary	Amount (kg)	5700	kg	Masskg
Summary	Amount (Nm3)	2.38597352766815	Nm3	VolumeNm3
Summary	Extra energy (kWh)	0	kWh	EnergykWh
Summary	Total Exergy	666.2412048528	kWh	EnergykWh
Species	NiO	119.7	kg	Masskg
Species	Fe2O3	1254	kg	Masskg
Species	CoO	4.56	kg	Masskg
Species	CuO	0.684	kg	Masskg
Species	Cr2O3	39.9	kg	Masskg
Species	SiO2	2223	kg	Masskg
Species	CaO	228	kg	Masskg
Species	Al2O3	282.15	kg	Masskg
Species	H2O	855	kg	Masskg
Species	MgO	693.006	kg	Masskg

Unit Name	Stream Name	Amount	Unit	Lca Equivalent	Lca Group
NiPigIronEF	Coke	356.65	kg	No Mapping	Not defined
NiPigIronEF	Limestone	869.41	kg	No Mapping	Not defined
NiPigIronEF	Infiltrate Air	128.67	kg	No Mapping	Not defined
NiPigIronEF	Power kWh	5300.47	kwh	No Mapping	Not defined

Fig. 4. "Input" streams info sheet extracted from flowsheet showing the laterite details.

The LCA streams sheets contain the HSC Sim stream names (as defined by the design engineer) and amounts, which must be mapped to the GaBi LCA equivalents on the GaBi database. The default is "No Mapping" which, unless changed, will exclude that stream from the evaluation. **Fig. 4** shows the details of the laterite input stream while **Fig. 5** shows the output and more specifically the pig iron stream. Please note that the exergy value is also given, which is very useful additional information for analyzing technology, reactors, plants, and systems.



Unit Name	Stream Name	Amount	Unit	Lca Equivalent	Lca Group	Main Product
NiPigIronEF	Slag	4279.05	kg	No Mapping	Not defined	☐
NiPigIronEF	Ni Pig Iron	1019.28	kg	No Mapping	Not defined	☑

Output Streams

Value Class	Name	Value	Unit Text	Unit Enum
Summary	Amount (kg)	1019.28377545331	kg	Masskg
Summary	Amount (Nm3)	0.150249149287767	Nm3	VolumeNm3
Summary	Extra energy (kWh)	0	kWh	EnergykWh
Summary	Total Exergy	257545.550861513	kWh	EnergykWh
Species	Si(l)	31.4964345332637	kg	Masskg
Species	Fe(l)	859.537992162226	kg	Masskg
Species	Cu(l)	0.540959117183395	kg	Masskg
Species	Cr(l)	0.272996766901068	kg	Masskg
Species	Ni(l)	84.6539423076923	kg	Masskg
Species	Co(l)	3.55049781132093	kg	Masskg
Species	P(l)	0	kg	Masskg
Species	C	39.2309527547227	kg	Masskg
Species		0	kg	Masskg
Element	C	39.2309527547227	kg	Masskg

Unit Name	Stream Name	Amount	Unit	Lca Equivalent	Lca Group	Main Product
NiPigIronEF	Offgas	1710.51	kg	No Mapping	Not defined	☐
NiPigIronEF	Fluedust	45.89	kg	No Mapping	Not defined	☐
NiPigIronEF	Heat Loss	200.00	kwh	No Mapping	Not defined	☐

Fig. 5. LCA Streams sheet for "Output," also marking the main product relative to which every flow is normalized.

49.3.2. Adding Manual Streams not Defined in the Process Simulation Model

Sometimes, during the LCI development via HSC Simulation, some missing streams may be identified. The best and recommended way is to add missing streams directly to the process simulation model. This typically would include all fugitive emissions, additional power, leakages from the system, etc. In some cases it is also appropriate to add streams for LCA purposes only. Adding these is done via the “Manual Streams” sheet, as depicted in **Fig. 6**.

For example, if general ancillary process electricity usage is not defined with its own stream in the process simulation model, then it can be defined via the manual streams dialog sheet. This can also be done for the output side. As shown in **Fig. 6**, the stream can be added (click on “Add new input stream” button at the bottom of the window), adding a name as well as the units and the amount for the flow that matches the data in the flowsheet as it is being simulated.

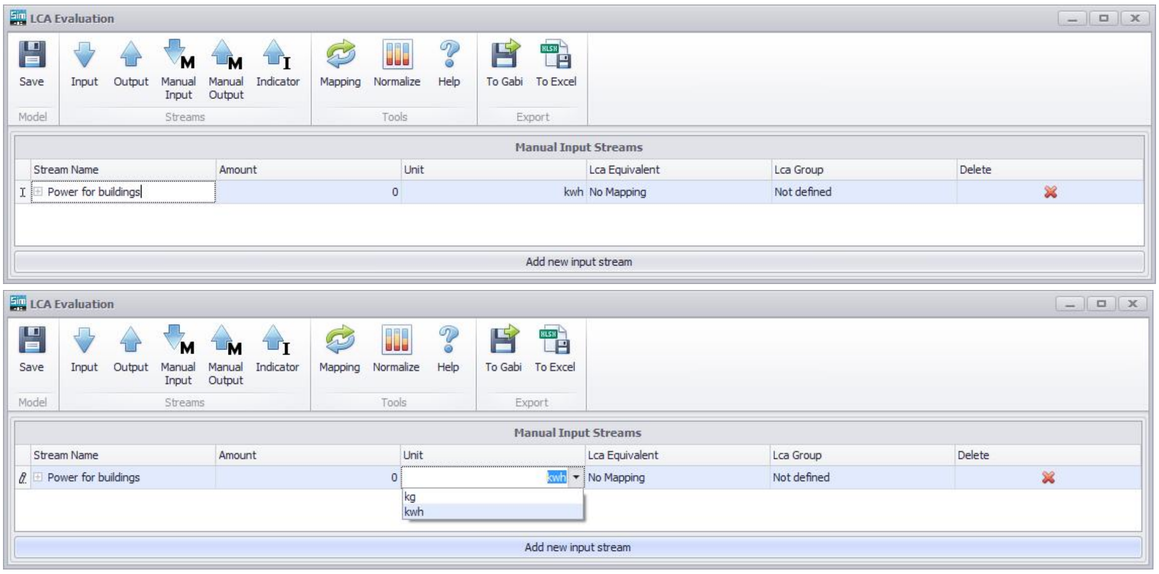


Fig. 6. LCA Manual Streams sheet for defining additional flows that do not appear in the simulation.

The key indicator sheet offers the possibility to examine how much of the compounds are released into the environment in the offgas or flue dust etc. This is a valuable part of the evaluation as a transparent analysis can be made of all the compounds that flow into the environment. **Fig. 7** shows all the indicator values and adds them together once they have been mapped as entering the environment. You can use the “*”' wildcard (**Table 1**) to capture more than a single compound, e.g. CO* will collect all CO and CO_2 etc. species, as defined in the model.

Table 1. Possible wildcard for compound definition

Wildcard	Description
*	Zero or more characters
?	Any single character
#	Any single digit (0-9)

You can type any compound in the sheet after having clicked on the Add new input stream bar at the bottom of the window. Some defaults are given. The compound definition may contain wildcards, as presented in **Table 1**. The LCA tool will automatically check if there are double counts of elements/compounds/species. A message box informs the user of double counting and will not add the compound to the list.

All the indicators which have some amount will be automatically added to the Manual Output streams list. If these emissions are to be excluded from the LCA analysis, the streams can be deleted manually by clicking the red cross.

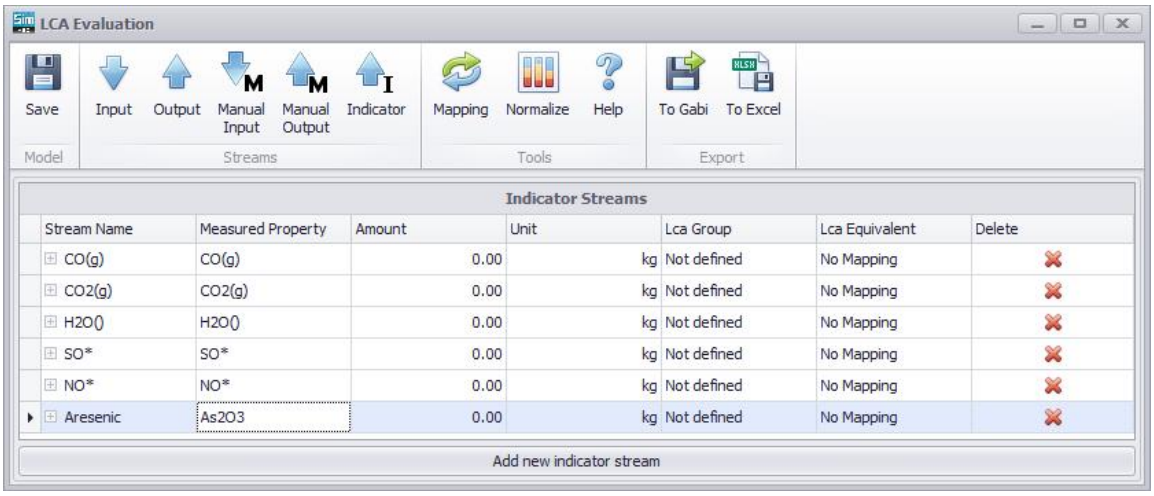


Fig. 7. Key Indicator sheet, showing the entry of a new compound that has to be tracked for environmental impact.

49.3.3. Mapping of Process Simulation Flows with GaBi Flow Definitions

In order to perform LCA calculations, all HSC streams have to be mapped to GaBi equivalents. All automatically included input and output streams have to be mapped but mapping of predefined manual streams are not mandatory. Non-mapped streams are discarded automatically. The mapping dialog is started by clicking the mapping button on the button menu. On the left side of the dialog window, all the HSC Sim process streams are given and the search tool for the GaBi database is on the right side. Stream mapping and selection is done by drag-and-drop from the GaBi side to the HSC side (see **Fig. 8**). The right side will be updated automatically if changes are made to that stream.

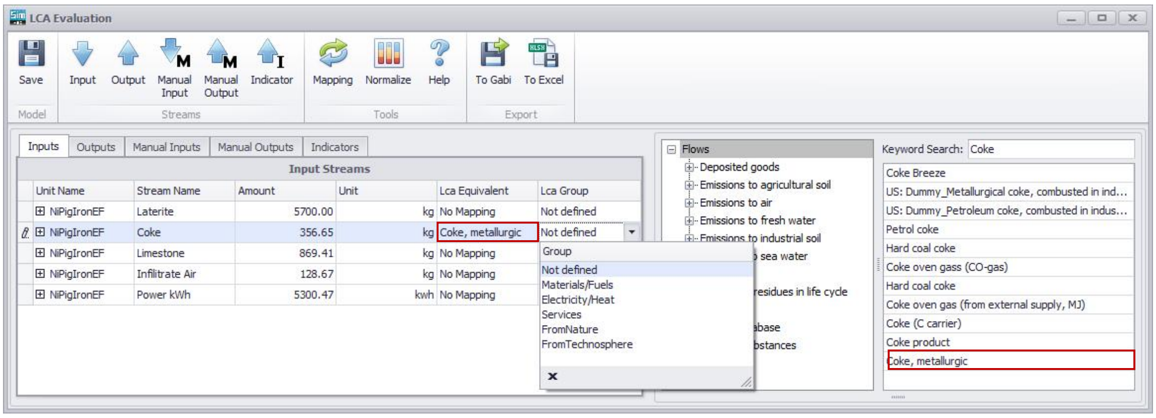


Fig. 8. Selecting a stream for mapping by drag-and-drop from the right into the LCA Equivalent box as shown in red. Please note that here you also have to select where this stream comes from, using the dropdown menu.

Selection of the flow group is always a very important step. The flow group defines the nature of the stream, i.e. where it comes and where it flows to. There are specific group types for input flows and output flows. The flow group is selected from the dropdown menu as shown in **Fig. 8**.

There are two possibilities to search for the LCA equivalent of each stream.

A keyword search is one option, during which the hits are listed below the search word (**Fig. 8**) and the second option is a tree view for manual searching (**Fig. 9**). In both cases, double click on the stream name to make a selection. With the keyword search, it is possible to limit the search by selecting some tree view node before the search, so that the search is performed under the selected node. All hits below that node will be presented. Also shown is the pulldown menu for the LCA Group (**Fig. 8**) and the possible places where it can flow to as selected, as shown in **Fig. 9**.

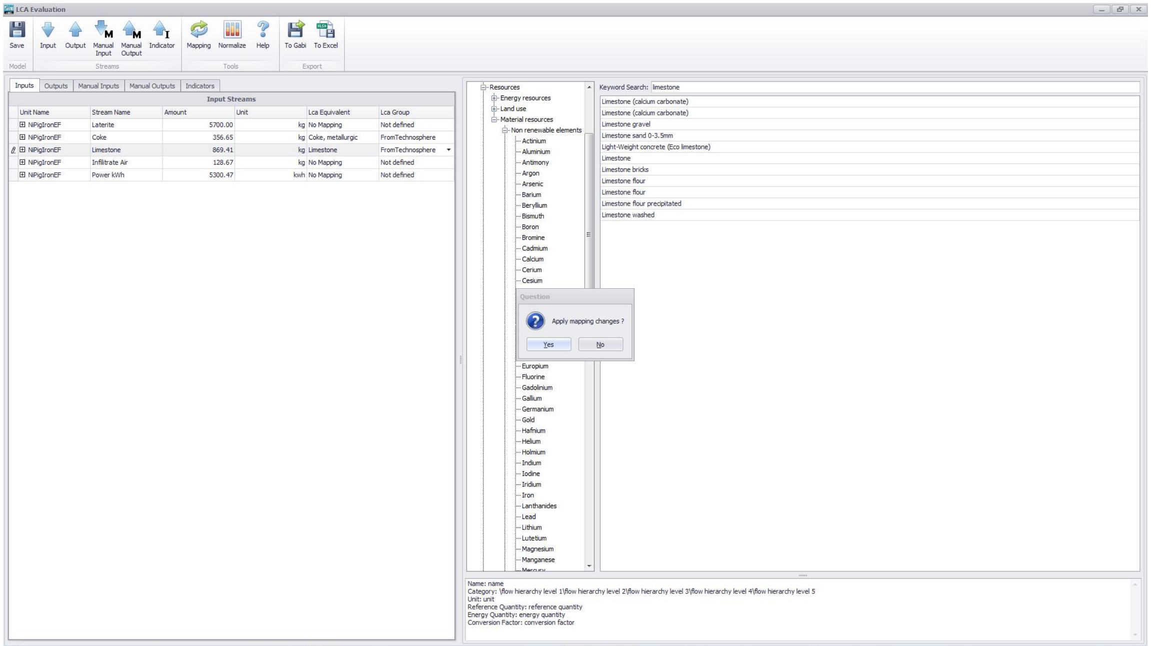


Fig. 9. LCA equivalent search from the GaBi database structure, selection of LCA Group. When navigating away you are asked to apply mapping.

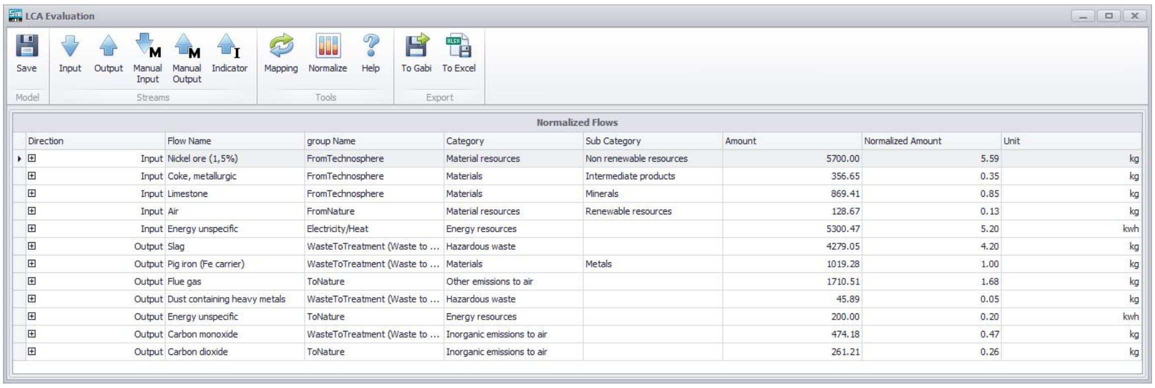
The stream description field shows the stream name, category and reference quantity, as shown at the bottom of **Fig. 9**. If changes are required, simply drag and drop a new GaBi equivalent or if something is to be omitted select Not defined from the pulldown menu. When navigating away from the page you will be prompted to apply the changes as shown in **Fig. 9**. All changes must always be saved to be effective.

49.3.4. Main Product Selection and Normalization of Data

Selection of the Main product is needed in order for normalization of the data to be performed. The Main product is always one of the output streams. No matter how many by-products there are, only one main product can be selected as all flows are normalized relative to this. This selection is made by checking the box, as shown in **Fig. 5**.

Normalize calculates how much of each flow is needed to obtain 1 kg of the main product. The Normalize button in the button menu executes normalization and the results are written in a new LCA normalized data sheet, which appears after the calculation, as shown in **Fig. 10**. The normalization sheet summarizes all the process LCA data and also provides a good opportunity to check the data validity. All the same mappings are combined in one stream and unmapped streams are not included in the summary. If, for example, more than one stream is mapped with the same GaBi data “Air”, all Air LCA Equivalents will be added to create one stream.

This normalization sheet (**Fig. 10**) also provides a complete overview of all the flows, which thus provides an excellent black box summary of the complete simulation, producing a complete and consistent mass and energy balance. As only mapped inputs and outputs are considered and no internal flows, the black box does not reveal any proprietary process detail, making it ideal for benchmarking processes, inclusion in environmental databases, etc.



Direction	Flow Name	group Name	Category	Sub Category	Amount	Normalized Amount	Unit
Input	Nickel ore (1,5%)	FromTechnosphere	Material resources	Non renewable resources	5700.00	5.59	kg
Input	Coke, metallurgic	FromTechnosphere	Materials	Intermediate products	356.65	0.35	kg
Input	Limestone	FromTechnosphere	Materials	Minerals	869.41	0.85	kg
Input	Air	FromNature	Material resources	Renewable resources	128.67	0.13	kg
Input	Energy unspecific	Electricity/Heat	Energy resources		5300.47	5.20	kwh
Output	Slag	WasteToTreatment (Waste to ...	Hazardous waste		4279.05	4.20	kg
Output	Pig iron (Fe carrier)	WasteToTreatment (Waste to ...	Materials	Metals	1019.28	1.00	kg
Output	Flue gas	ToNature	Other emissions to air		1710.51	1.68	kg
Output	Dust containing heavy metals	WasteToTreatment (Waste to ...	Hazardous waste		45.89	0.05	kg
Output	Energy unspecific	ToNature	Energy resources		200.00	0.20	kwh
Output	Carbon monoxide	WasteToTreatment (Waste to ...	Inorganic emissions to air		474.18	0.47	kg
Output	Carbon dioxide	ToNature	Inorganic emissions to air		261.21	0.26	kg

Fig. 10. A complete normalized data set defining as a black box the complete process, flowsheet or system.

49.3.5. Exporting as an Ecospold File to GaBi and as an Excel File

The To GaBi exporting menu button writes an Ecospold version 1.0 XML file. The exported file contains metadata, which provides general process information as required by the LCA methodology. Metadata information is entered in the Process Information window and needs to be completed before exporting (**Fig. 11**). Stream details are taken from the normalization sheet.

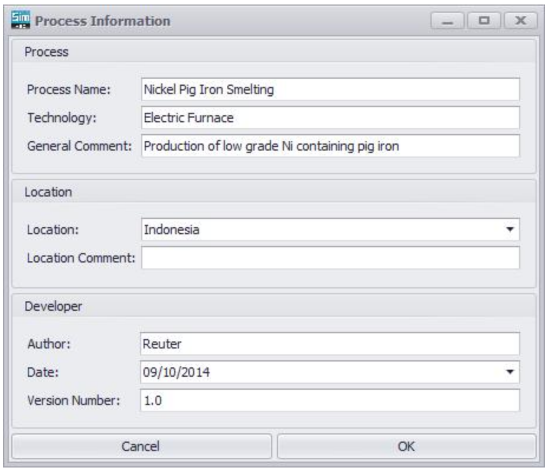


Fig. 11. Process Info dialog for entering process detail.

It is not mandatory to complete all process information fields but it is worth filling well in order to export the process in a form that is best usable in GaBi. After completion of the process information, save it by clicking. Process info can also be used without the LCA tool to describe the process well, hence providing a good summary for use in a process design.

The To GaBi exporting button is found on the button menu, to the right of the Normalize button. If normalization has not been done, the LCA tool will automatically ask you to perform normalization first. Exporting opens a file search dialog where the location and

name of the exported file is defined/entered. The “Export done” popup window will inform the user when the export is ready, as shown by **Fig. 12**.

There is also an option to export the information to Excel, which can be used as an input for other applications, reports, publications etc. as shown in **Fig. 13**.

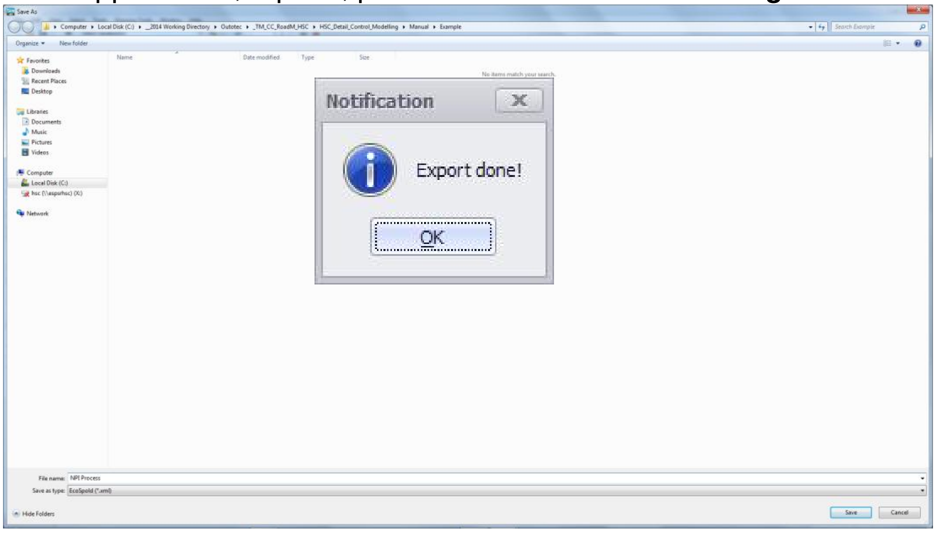


Fig. 12. Selection of export directory and file name.

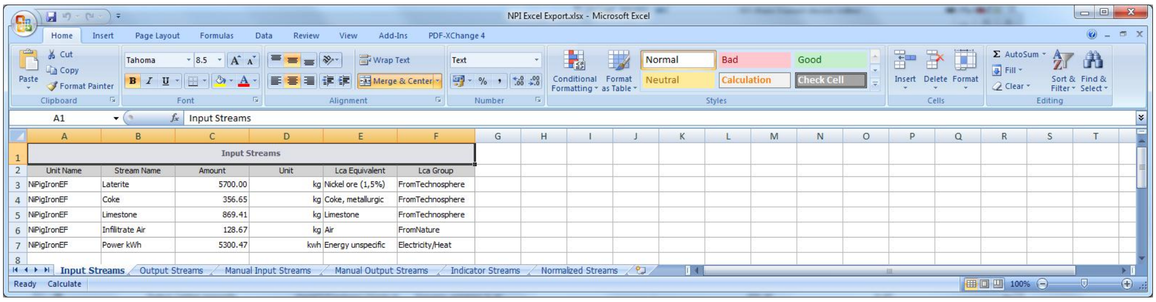


Fig. 13. The Excel export of all the information for further use by other software.

49.3.6. Importing a Process to GaBi and Further Analysis in the GaBi Plan Functionality

GaBi software is 3rd party LCA software and not part of HSC Chemistry software (http://tutorials.gabi-software.com/)[4]. Extending the GaBi process database is possible by selecting Database→Import→Ecospold, producing functional GaBi processes.

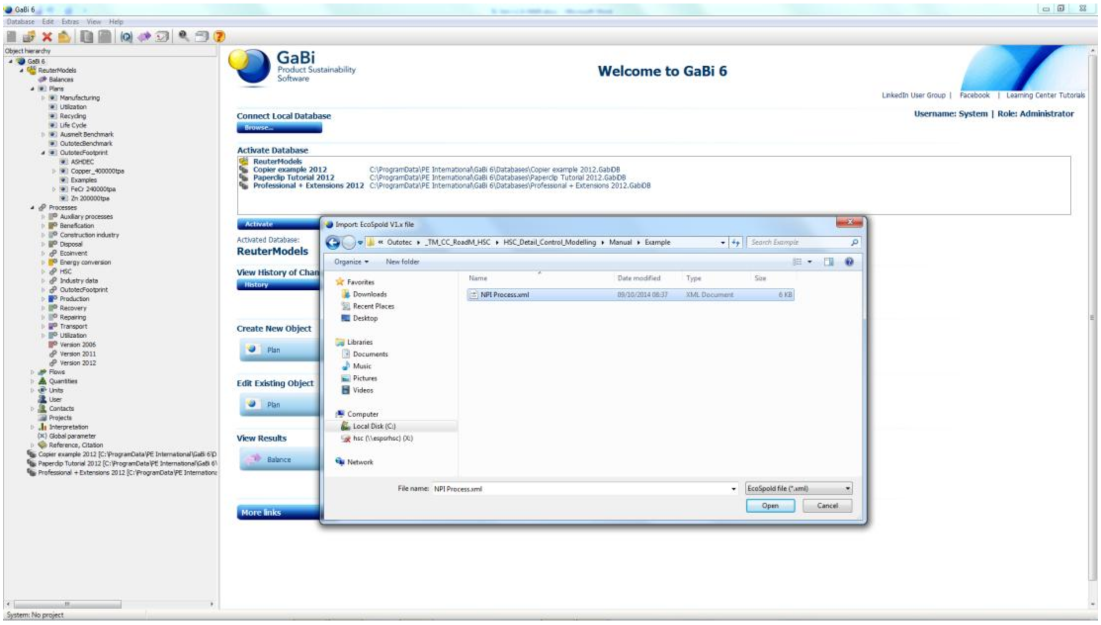


Fig. 14. Importing a new process to the GaBi database from the directory into which the XML file was exported.

A file searching window opens for the exported HSC Sim file search, as shown in **Fig. 14**. File selection first opens the process summary, where the user is also informed of the process export path in the GaBi process tree. **Fig. 14** lists all the flows and amounts and if this summary is OK, the final import can be started by clicking the green play button. At the end of this import, a log file popup appears in GaBi that informs the user whether the import was successful or not. The log file can be closed without saving in GaBi.

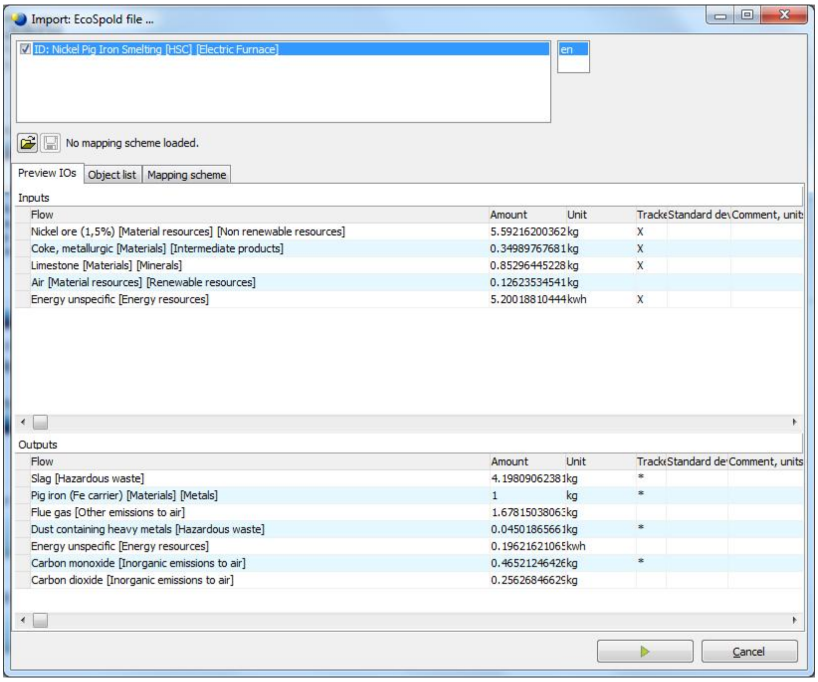


Fig. 15. Process summary presented during import as a check before clicking on the play button to complete the import.

The new process is available in GaBi Processes under the HSC folder. This HSC Sim generated process can now be used in the new LCA plans together with all other GaBi processes, functionality and an impact assessment performed as shown in **Fig. 17**.

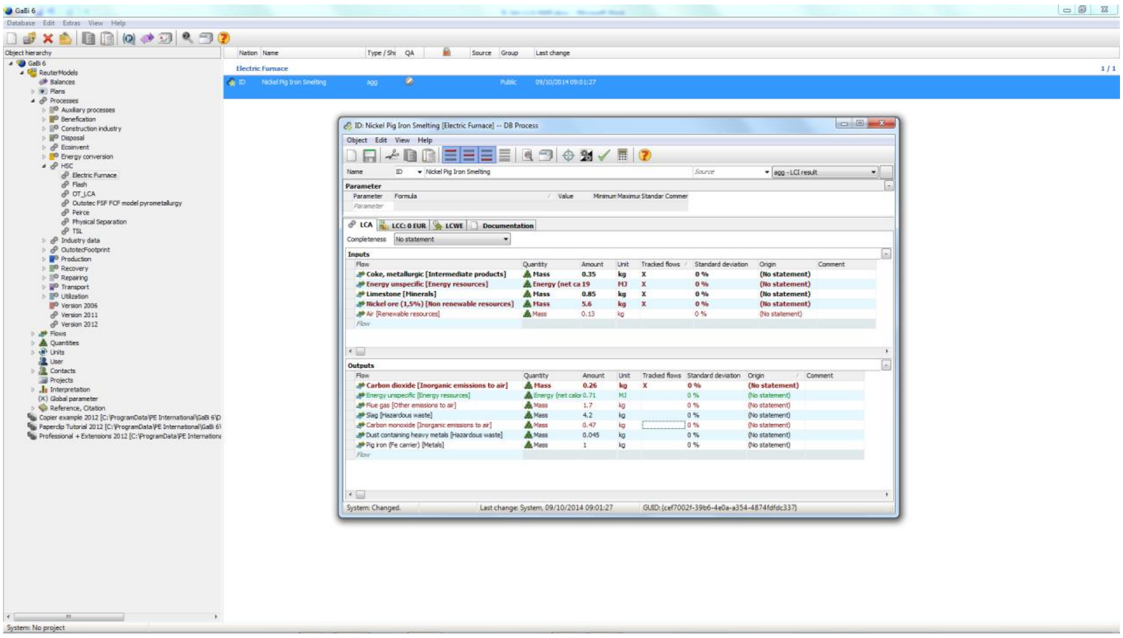


Fig. 16. New process located in Processes folder under the HSC node.

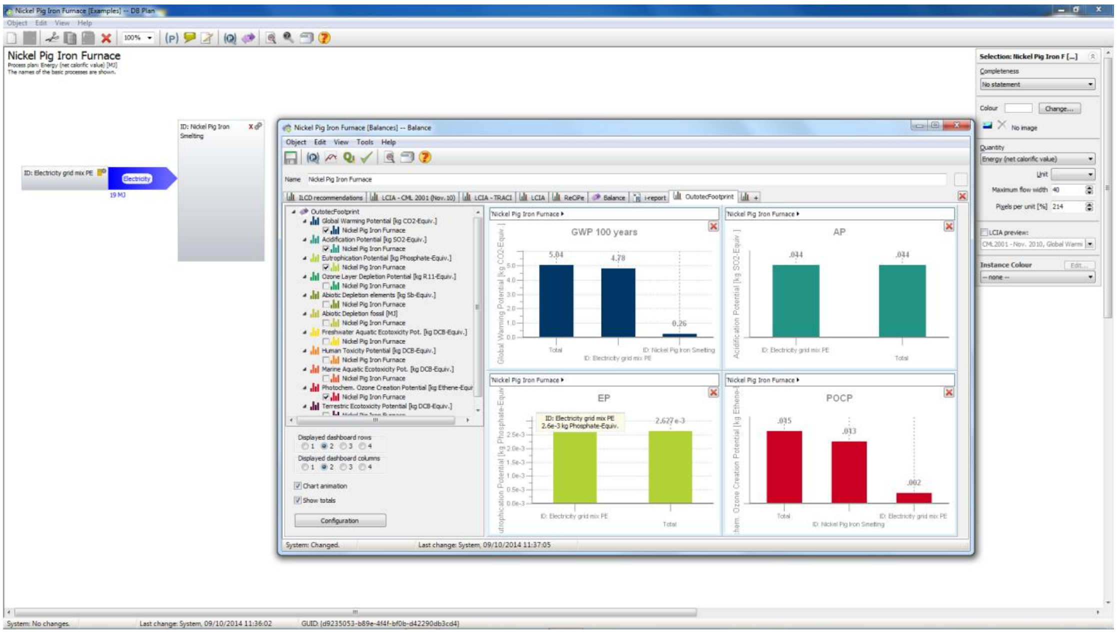


Fig. 17. The imported process can now be linked to other GaBi processes, e.g. energy and the calculated environmental impacts.

49.4. Bibliography

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